Access DB# 164848

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Sin J. Lee Examiner #: 76060 Date: 9-6-2005
Art Unit: 1752 Phone Number 30 2-1333 Serial Number: 10/781,862
Mail Box and Bldg/Room Location: 9D66 (Rem.) Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: P/Z. Lee B76.

Inventors (please provide full names):

Earliest Priority Filing Date:

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

P/Z. search for a compound of Cl. #6

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STAFF USE ONLY	Type of Search		Vendors and cost where applicable	
Searcher: LH	NA Sequence (#)		STN	$87.56
Searcher Phone #:	AA Sequence (#)		Dialog	
Searcher Location:	Structure (#)	1	Questel/Orbit	
Date Searcher Picked Up:	Bibliographic		Dr.Link	
Date Completed: 9/23/05	Litigation		Lexis/Nexis	
Searcher Prep & Review Time: 1.5	Fulltext		Sequence Systems	
Clerical Prep Time: 30	Patent Family		WWW/Internet	
Online Time: 30	Other		Other (specify)	

PTO-1590 (8-01)

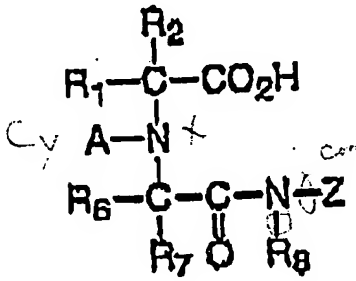
A represents an aromatic group or a heterocyclic group,

R^1 and R^2 each independently represents a hydrogen atom or a monovalent substituent, provided that R^1 and R^2, either one of R^1 and R^2 and X^1, either one of R^1 and R^2 and A, or A and X^1 may be taken together to form a ring structure,

X^1 represents a divalent connection group selected from -O-, -S-, $-SO_2-$, -NH-, $-N(R^3)-$, $-CH_2-$, $-CH(R^4)-$, and $-C(R^4)(R^5)-$, and

R^3, R^4, and R^5 each independently represents a hydrogen atom or a monovalent substituent.

6. (original): The polymerizable composition according to claim 1, wherein the compound (A) is a compound represented by the following formula:



wherein

A represents an aromatic group or a heterocyclic group,

R^1, R^2, R^6, R^7 and R^8 each independently represents a hydrogen atom or a monovalent substituent, provided that R^1 and R^2, either one of R^1 and R^2 and A, or R^8 and Z may be taken together to form a ring structure,

and

Z represents a monovalent substituent.

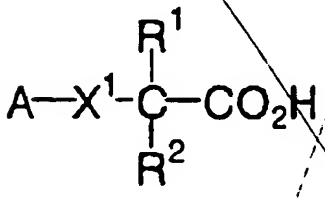
7. (original): A polymerizable composition comprising:

(A-1) a monocarboxylic acid compound represented by the following formula (I-2);

(B) a radical initiator;

(C) a compound having at least one ethylenically unsaturated bond; and

(D) an infrared ray absorber:



(1-2)

wherein

A represents an aromatic group or a heterocyclic group,

R^1 and R^2 each independently represents a hydrogen atom or a monovalent substituent, provided that R^1 and R^2, either one of R^1 and R^2 and X^1, either one of R^1 and R^2 and A, or A and X^1 may be taken together to form a ring structure,

X^1 represents a divalent connection group selected from -O-, -S-, $-SO_2-$, -NH-, $-N(R^3)-$, $-CH_2-$, $-CH(R^4)-$, and $-C(R^4)(R^5)-$, and

R^3, R^4, and R^5 each independently represents a hydrogen atom or a monovalent substituent.

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=> d his ful

     (FILE 'HOME' ENTERED AT 08:44:39 ON 22 SEP 2005)

     FILE 'HCAPLUS' ENTERED AT 08:44:49 ON 22 SEP 2005
                E US20050106495/PN
L1            1 SEA ABB=ON  PLU=ON  US20050106495/PN
                D ALL
                SEL L1 RN

     FILE 'REGISTRY' ENTERED AT 08:46:20 ON 22 SEP 2005
L2           42 SEA ABB=ON  PLU=ON  (103-01-5/BI OR 1137-73-1/BI OR
                122-59-8/BI OR 161555-27-7/BI OR 35676-11-0/BI OR
                3959-23-7/BI OR 60085-74-7/BI OR 62952-26-5/BI OR
                6915-15-7/BI OR 743422-66-4/BI OR 743422-67-5/BI OR
                743422-68-6/BI OR 743422-69-7/BI OR 743422-70-0/BI OR
                743422-71-1/BI OR 743422-72-2/BI OR 743422-73-3/BI OR
                743422-74-4/BI OR 743422-75-5/BI OR 743422-76-6/BI OR
                743422-77-7/BI OR 743422-78-8/BI OR 743422-79-9/BI OR
                743422-80-2/BI OR 743422-81-3/BI OR 743422-82-4/BI OR
                743422-83-5/BI OR 743422-84-6/BI OR 743422-85-7/BI OR
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                743422-90-4/BI OR 743422-92-6/BI OR 743422-93-7/BI OR
                743422-96-0/BI OR 743422-98-2/BI OR 743422-99-3/BI OR
                743423-00-9/BI OR 743423-01-0/BI OR 743423-02-1/BI OR
                743423-03-2/BI)
                D SCAN

     FILE 'LREGISTRY' ENTERED AT 08:53:28 ON 22 SEP 2005
L3              STR

     FILE 'REGISTRY' ENTERED AT 09:00:25 ON 22 SEP 2005
L4           50 SEA SSS SAM L3

     FILE 'LREGISTRY' ENTERED AT 09:01:22 ON 22 SEP 2005
L5              STR L3

     FILE 'REGISTRY' ENTERED AT 09:02:41 ON 22 SEP 2005
                D SCAN L2

     FILE 'LREGISTRY' ENTERED AT 09:06:54 ON 22 SEP 2005
L6              STR L5

     FILE 'REGISTRY' ENTERED AT 09:19:04 ON 22 SEP 2005
                D QUE STAT L5
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L7              STR L5
L8              STR L6

     FILE 'REGISTRY' ENTERED AT 09:23:12 ON 22 SEP 2005
L9           50 SEA SSS SAM L7
L10           1 SEA SSS SAM L8
                D SCAN
L11             SCR 1918
L12          50 SEA SSS SAM L7 NOT L11
                D SCAN L10
L13             SCR 1841
L14          50 SEA SSS SAM L7 NOT L13
L15             SCR 1918 OR 1841
L16          50 SEA SSS SAM L7 NOT L15
L17             SCR 1312
L18          50 SEA SSS SAM L7 AND L17
L19          50 SEA SSS SAM L7 AND L17 NOT L13
L20          50 SEA SSS SAM L7 AND L17 NOT L15
L21             SCR 1312 OR 2036 OR 2021
L22             SCR 1841 OR 2016 OR 1964 OR 1921 OR 1957 OR 1931 OR 1919
L23          50 SEA SSS SAM L7 AND L21 NOT L22
                D QUE STAT
                D QUE STAT L10

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L24             STR L7

     FILE 'REGISTRY' ENTERED AT 10:04:41 ON 22 SEP 2005
L25          50 SEA SSS SAM L24 AND L21 NOT L22
                D QUE STAT
L26             SCR 1841 OR 1918 OR 2016
L27          50 SEA SSS SAM L24 AND L21 NOT L26
                D QUE STAT
L28             SCR 1312 AND 1838
L29          50 SEA SSS SAM L24 AND L28
L30          50 SEA SSS SAM L24 AND L28 NOT L26
L31          50 SEA SSS SAM L24 AND L28 NOT L22
                D QUE STAT L31
                D QUE STAT L30
L32             SCR 1526 AND 1838
L33          50 SEA SSS SAM L24 AND L32
L34          50 SEA SSS SAM L24 AND L32 NOT L22
L35          50 SEA SSS SAM L24 AND L32 NOT L26
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     FILE 'REGISTRY' ENTERED AT 11:07:10 ON 22 SEP 2005
L37          50 SEA SSS SAM L36 AND L32 NOT L22
L38             SCR 1841 OR 2016 OR 1964 OR 1921 OR 1957 OR 1931 OR 1919
L39          50 SEA SSS SAM L36 AND L32 NOT L38
                D QUE STAT
                D SAV
L40             SCR 1841 OR 2016 OR 1964 OR 1921 OR 1957 OR 1931 OR 1919
L41          50 SEA SSS SAM L36 AND L32 NOT L40
                D QUE STAT L39
                D QUE STAT
                D QUE L40
                D QUE L38
L42             SCR 2040
L43          50 SEA SSS SAM L36 AND L32 NOT (L42 OR L38)
L44             SCR 2077
L45          50 SEA SSS SAM L36 AND L32 NOT (L42 OR L38 OR L44)
L46      145388 SEA SSS FUL L36 AND L32 NOT (L42 OR L38 OR L44)

                SAV TEMP L46 LEE862/A

     FILE 'HCAPLUS' ENTERED AT 11:24:01 ON 22 SEP 2005

     FILE 'REGISTRY' ENTERED AT 11:24:11 ON 22 SEP 2005
L47          37 SEA ABB=ON  PLU=ON  L2 AND L46

     FILE 'HCAPLUS' ENTERED AT 11:24:38 ON 22 SEP 2005
L48      285971 SEA ABB=ON  PLU=ON  L46
L49        2743 SEA ABB=ON  PLU=ON  L47
L50       36476 SEA ABB=ON  PLU=ON  DECARBOXYLAT?
L51        4455 SEA ABB=ON  PLU=ON  L48 AND L50
L52             QUE ABB=ON  PLU=ON  POLYMERIZ? OR POLYMERIS? OR POLYM#
                OR CURE# OR CURING# OR DIGEST? OR CROSSLINK? OR CROSS(W)L
                INK? OR VULCANIZ? OR VITRIF? OR GEL?
L53         211 SEA ABB=ON  PLU=ON  L51 AND L52
L54      516279 SEA ABB=ON  PLU=ON  POLYMERIZ?
L55         111 SEA ABB=ON  PLU=ON  L54 AND L53
L56        6926 SEA ABB=ON  PLU=ON  (INFRARED OR IR)(2A)ABSORB?
L57           2 SEA ABB=ON  PLU=ON  L56 AND L55
                D SCAN
L58           3 SEA ABB=ON  PLU=ON  L56 AND L51
L59           3 SEA ABB=ON  PLU=ON  L57 OR L58
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L60	52	SEA ABB=ON	PLU=ON	L48 AND L56
L61	656336	SEA ABB=ON	PLU=ON	INFRARED OR IR
L62	11	SEA ABB=ON	PLU=ON	L61 AND L55
L63	19	SEA ABB=ON	PLU=ON	L61 AND L53
L64	52	SEA ABB=ON	PLU=ON	L56 AND L48
L65	159	SEA ABB=ON	PLU=ON	L61 AND L51
		D QUE L52		
L66	19758	SEA ABB=ON	PLU=ON	RADICAL(2A)INIT?
L67	12	SEA ABB=ON	PLU=ON	L66 AND L51
L68	5	SEA ABB=ON	PLU=ON	L66 AND L55
L69	1	SEA ABB=ON	PLU=ON	L66 AND L59
		D SCAN		
L70	470272	SEA ABB=ON	PLU=ON	74/SC,SX
L71	9	SEA ABB=ON	PLU=ON	L70 AND L55
L72	13	SEA ABB=ON	PLU=ON	L70 AND L53
L73	17	SEA ABB=ON	PLU=ON	L59 OR L68 OR L69 OR L71 OR L72
L74	26	SEA ABB=ON	PLU=ON	L73 OR L62
L75	34	SEA ABB=ON	PLU=ON	L74 OR L63
L76	1	SEA ABB=ON	PLU=ON	L75 AND L1
L77	65	SEA ABB=ON	PLU=ON	L49 AND L50
L78	62	SEA ABB=ON	PLU=ON	L77 NOT L75
L79	7	SEA ABB=ON	PLU=ON	L77 AND L52
L80	1	SEA ABB=ON	PLU=ON	L79 AND L56
L81	1	SEA ABB=ON	PLU=ON	L77 AND L56
L82	3	SEA ABB=ON	PLU=ON	L77 AND L66
L83	7	SEA ABB=ON	PLU=ON	L77 AND L70
L84	12	SEA ABB=ON	PLU=ON	(L79 OR L80 OR L81 OR L82 OR L83)
L85	43	SEA ABB=ON	PLU=ON	L75 OR L84
L86	31	SEA ABB=ON	PLU=ON	L85 NOT L84
L87	137411	SEA ABB=ON	PLU=ON	DEHYDRAT? OR DE(W)HYDRAT?
L88	2911	SEA ABB=ON	PLU=ON	L87 AND L48
L89	279	SEA ABB=ON	PLU=ON	L88 AND L50
L90	17	SEA ABB=ON	PLU=ON	L89 AND L52
L91	1	SEA ABB=ON	PLU=ON	L89 AND L56
L92	16	SEA ABB=ON	PLU=ON	L89 AND L61
L93	1	SEA ABB=ON	PLU=ON	L89 AND L66
L94	2	SEA ABB=ON	PLU=ON	L89 AND L70
L95	31	SEA ABB=ON	PLU=ON	(L90 OR L91 OR L92 OR L93 OR L94)
L96	70	SEA ABB=ON	PLU=ON	L95 OR L85
L97	279	SEA ABB=ON	PLU=ON	L88 AND L50
L98	17	SEA ABB=ON	PLU=ON	L97 AND L52
L99	1	SEA ABB=ON	PLU=ON	L98 AND L56
L100	1	SEA ABB=ON	PLU=ON	L98 AND L66
L101	1	SEA ABB=ON	PLU=ON	L98 AND L70
L102	1	SEA ABB=ON	PLU=ON	L97 AND L56

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L103          1 SEA ABB=ON  PLU=ON  L97 AND L66
L104          2 SEA ABB=ON  PLU=ON  L97 AND L70
L105      19455 SEA ABB=ON  PLU=ON  L48 AND L52
L106         27 SEA ABB=ON  PLU=ON  L105 AND L56
L107          6 SEA ABB=ON  PLU=ON  L106 AND L66
L108         23 SEA ABB=ON  PLU=ON  L106 AND L70
                D QUE STAT
L109         16 SEA ABB=ON  PLU=ON  L49 AND L56
L110          3 SEA ABB=ON  PLU=ON  L109 AND L66
L111         14 SEA ABB=ON  PLU=ON  L109 AND L70
L112          9 SEA ABB=ON  PLU=ON  L89 AND L54
L113          9 SEA ABB=ON  PLU=ON  L95 AND L54
L114         47 SEA ABB=ON  PLU=ON  (L98 OR L99 OR L100 OR L101 OR L102
                OR L103 OR L104) OR (L106 OR L107 OR L108 OR L109 OR
                L110 OR L111 OR L112 OR L113)
L115         30 SEA ABB=ON  PLU=ON  L114 AND L54
L116         71 SEA ABB=ON  PLU=ON  L115 OR L85
L117         10 SEA ABB=ON  PLU=ON  L112 OR (L100 OR L101 OR L102 OR
                L103 OR L104)
L118         15 SEA ABB=ON  PLU=ON  L117 OR L107 OR L110 OR L113
L119         57 SEA ABB=ON  PLU=ON  L118 OR L85
L120         68 SEA ABB=ON  PLU=ON  L119 OR L111
L121         35 SEA ABB=ON  PLU=ON  L49 AND L87
L122          5 SEA ABB=ON  PLU=ON  L121 AND L52
L123          1 SEA ABB=ON  PLU=ON  L121 AND L54
L124          1 SEA ABB=ON  PLU=ON  L121 AND L56
L125          1 SEA ABB=ON  PLU=ON  L121 AND L66
L126          2 SEA ABB=ON  PLU=ON  L121 AND L70
L127          5 SEA ABB=ON  PLU=ON  (L122 OR L123 OR L124 OR L125 OR
                L126)
L128         60 SEA ABB=ON  PLU=ON  L127 OR L119
L129         71 SEA ABB=ON  PLU=ON  L128 OR L120
                D QUE STAT L128
                D L128 1-60 CBIB ABS HITSTR HITIND

     FILE 'REGISTRY' ENTERED AT 12:27:28 ON 22 SEP 2005
                D QUE STAT L8
L130          2 SEA SUB=L46 SSS SAM L8
                D SCAN
L131         29 SEA SUB=L46 SSS FUL L8

     FILE 'HCAPLUS' ENTERED AT 12:29:05 ON 22 SEP 2005
L132         14 SEA ABB=ON  PLU=ON  L131

     FILE 'CAOLD' ENTERED AT 12:29:25 ON 22 SEP 2005
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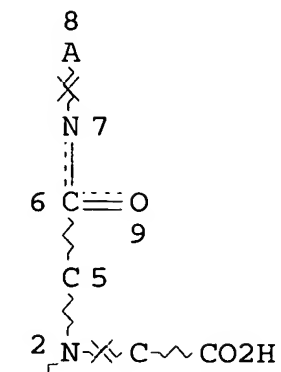
L133 1 SEA ABB=ON PLU=ON L131

=> => => d que stat l132
L8 STR



NODE ATTRIBUTES:
NSPEC IS RC AT 2
NSPEC IS RC AT 7
NSPEC IS RC AT 8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
L32 SCR 1526 AND 1838
L36 STR

Cy G1 CH CO2H
5 2 3 4

VAR G1=C/N/O/S
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M4-X14 C AT 5

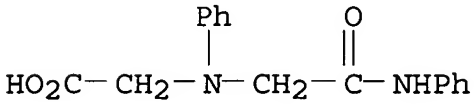
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 4

STEREO ATTRIBUTES: NONE
L38 SCR 1841 OR 2016 OR 1964 OR 1921 OR 1957 OR 1931 OR 1919 O
R 1995
L42 SCR 2040
L44 SCR 2077
L46 145388 SEA FILE=REGISTRY SSS FUL L36 AND L32 NOT (L42 OR L38 OR
L44)
L131 29 SEA FILE=REGISTRY SUB=L46 SSS FUL L8
L132 14 SEA FILE=HCAPLUS ABB=ON PLU=ON L131

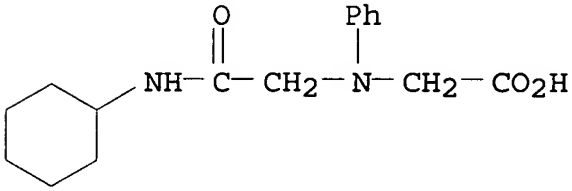
=> d l132 1-14 cbib abs hitstr hitind

L132 ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
2005:660755 Document No. 143:142810 IR-laser-sensitive
photopolymerizable compositions, and negative-working photoimaging
materials for various uses including printing plates. Fujimaki,
Kazuhiro (Fuji Photo Film Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho
JP 2005202314 A2 20050728, 84 pp. (Japanese). CODEN: JKXXAF.
APPLICATION: JP 2004-10832 20040119.
AB The compns. contain monocarboxylic acids, polycarboxylic acids,
IR-absorbing agents, radical polymerization initiators, and ethylenic
monomers, wherein the monocarboxylic acids and/or polycarboxylic
acids bear groups expressed by XC(R1)(R2)CO2H [X = O, S, SO2, CO,
NR3; R1-3 = H, monovalent nonmetallic substituent; R1 and R2, or R3
and R1 or R2 may form a ring]. Also claimed are the photoimaging
materials containing the compns. on supports. The carboxylic acids
work
as stabilizer for the polymerization initiators without causing drop
in
sensitivity of the compns. themselves in long-period storage. Thus,
a presensitized lithog. plate was manufactured by using the
composition containing
N-phenyliminodiacetic acid monoaniline amide.
IT **743422-98-2P**
RL: IMF (Industrial manufacture); MOA (Modifier or additive use);
TEM (Technical or engineered material use); PREP (Preparation); USES
(Uses)
(stabilizer for polymerization catalyst; photopolymerizable
composition
containing mono- and polycarboxylic acids as polymerization
catalyst

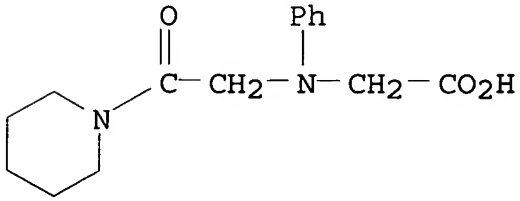
stabilizers)
RN 743422-98-2 HCAPLUS
CN Glycine, N-[2-oxo-2-(phenylamino)ethyl]-N-phenyl- (9CI) (CA INDEX NAME)



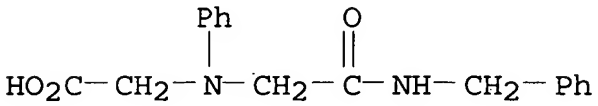
IT **743423-02-1 858967-70-1 858967-73-4**
RL: MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)
(stabilizer for polymerization catalyst; photopolymerizable composition
containing mono- and polycarboxylic acids as polymerization catalyst
stabilizers)
RN 743423-02-1 HCAPLUS
CN Glycine, N-[2-(cyclohexylamino)-2-oxoethyl]-N-phenyl- (9CI) (CA INDEX NAME)



RN 858967-70-1 HCAPLUS
CN Glycine, N-[2-oxo-2-(1-piperidinyl)ethyl]-N-phenyl- (9CI) (CA INDEX NAME)



RN 858967-73-4 HCAPLUS
CN Glycine, N-[2-oxo-2-[(phenylmethyl)amino]ethyl]-N-phenyl- (9CI) (CA INDEX NAME)



IC ICM G03F007-004
ICS C08F002-44; G03F007-00
CC 74-6 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 25, 38
IT 612-42-0P **743422-98-2P**
RL: IMF (Industrial manufacture); MOA (Modifier or additive use); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(stabilizer for polymerization catalyst; photopolymerizable composition
containing mono- and polycarboxylic acids as polymerization catalyst
stabilizers)
IT 88-99-3, 1,2-Benzenedicarboxylic acid, uses 103-01-5 4282-31-9, 2,5-Thiophenedicarboxylic acid 25395-22-6 87964-30-5
743423-02-1 858967-70-1 858967-73-4
858967-80-3 858967-83-6
RL: MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)
(stabilizer for polymerization catalyst; photopolymerizable composition
containing mono- and polycarboxylic acids as polymerization catalyst
stabilizers)

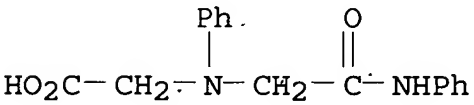
L132 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
2005:259485 Document No. 142:345190 Photosensitive composition and lithographic printing plate precursor using the same. Yanaka, Hiromitsu; Goto, Takahiro (Fuji Photo Film Co., Ltd., Japan). U.S. Pat. Appl. Publ. US 2005064331 A1 20050324, 34 pp. (English). CODEN: USXXCO. APPLICATION: US 2004-947260 20040923. PRIORITY: JP 2003-331528 20030924.
AB A photosensitive composition comprises (A) polymerizable compound A{O[(CH(R1)CH(R2))mO]nC(O)C(R3):CH2}p (R1-3 = H, Me; A = polyhydric

alc. residue, polyhydric phenol residue; m = 1-6; n = 1-20; p = 1-6), (B) an IR absorber, and (C) an onium salt.

IT **743422-98-2**
RL: MOA (Modifier or additive use); USES (Uses)
(photosensitive composition for lithog. printing plate precursor)

RN 743422-98-2 HCAPLUS

CN Glycine, N-[2-oxo-2-(phenylamino)ethyl]-N-phenyl- (9CI) (CA INDEX NAME)



IC ICM G03C001-492
ICS G03C001-005; G03F007-26

INCL 430270100; 430302000; 430627000

CC 74-6 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

IT 183745-11-1 **743422-98-2** 848489-55-4
RL: MOA (Modifier or additive use); USES (Uses)
(photosensitive composition for lithog. printing plate precursor)

L132 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

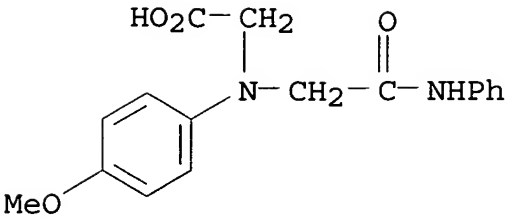
2005:140645 Document No. 142:228773 Lithographic printing plate precursor and lithographic printing method. Sonokawa, Koji (Japan). U.S. Pat. Appl. Publ. US 2005037282 A1 20050217, 31 pp. (English). CODEN: USXXCO. APPLICATION: US 2004-917354 20040813. PRIORITY: JP 2003-293814 20030815.

AB A lithog. printing plate precursor comprises: a support; and an image recording layer containing (A) an IR absorbing agent, (B) a polymerization initiator, (C) a polymerizable compound and (D) a compound having a carboxylate group and being removable with at least one of a printing ink and a fountain solution

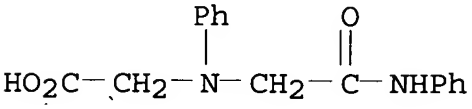
IT **35676-11-0 743422-98-2**
RL: TEM (Technical or engineered material use); USES (Uses)
(compound having a carboxylate group; lithog. printing plate precursor containing)

RN 35676-11-0 HCAPLUS

CN Glycine, N-(4-methoxyphenyl)-N-[2-oxo-2-(phenylamino)ethyl]- (9CI) (CA INDEX NAME)



RN 743422-98-2 HCAPLUS
CN Glycine, N-[2-oxo-2-(phenylamino)ethyl]-N-phenyl- (9CI) (CA INDEX NAME)



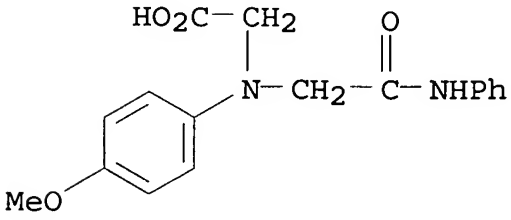
IC ICM G03F007-00
INCL 430270100; 430302000
CC 74-6 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
IT 103-01-5 122-59-8 334-48-5, Decanoic acid 528-44-9, 1,2,4-Benzenetricarboxylic acid 1137-73-1 3959-23-7 4282-31-9, 2,5-Thiophenedicarboxylic acid 16024-56-9 16024-58-1 **35676-11-0** 161555-27-7 743422-80-2 743422-81-3 743422-82-4 743422-92-6 **743422-98-2** 844499-45-2 844499-46-3
RL: TEM (Technical or engineered material use); USES (Uses) (compound having a carboxylate group; lithog. printing plate precursor containing)

L132 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
2004:700261 Document No. 141:215685 Polymerizable composition and lithographic printing plate precursor. Fujimaki, Kazuhiro (Fuji Photo Film Co., Ltd., Japan). Eur. Pat. Appl. EP 1449651 A2 20040825, 96 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK. (English). CODEN: EPXXDW. APPLICATION: EP 2004-3844 20040220. PRIORITY: JP 2003-43087 20030220; JP 2003-194852 20030710.
AB A polymerizable composition comprises: (A) a compound which causes at least one of decarboxylation and dehydration by heat; (B) a radical initiator; (C) a compound having at least one ethylenically unsatd.

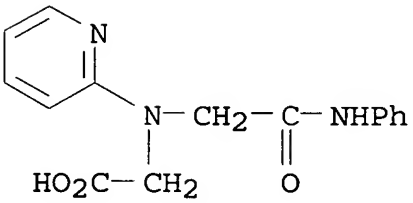
bond; and (D) an IR ray absorber and a lithog. printing plate precursor comprising a support and a recording layer comprising said polymerizable composition

IT **35676-11-0 743422-73-3 743422-98-2 743422-99-3 743423-00-9 743423-01-0 743423-02-1 743423-03-2**
RL: TEM (Technical or engineered material use); USES (Uses) (polymerizable composition and lithog. printing plate precursor containing)

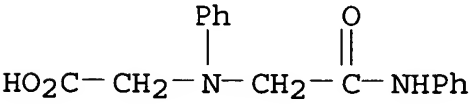
RN 35676-11-0 HCAPLUS
CN Glycine, N-(4-methoxyphenyl)-N-[2-oxo-2-(phenylamino)ethyl]- (9CI) (CA INDEX NAME)



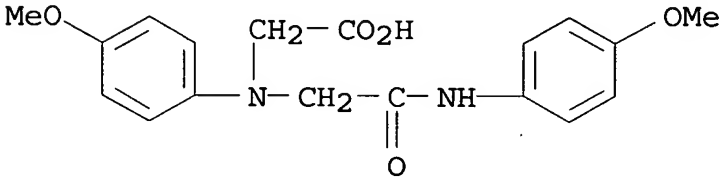
RN 743422-73-3 HCAPLUS
CN Glycine, N-[2-oxo-2-(phenylamino)ethyl]-N-2-pyridinyl- (9CI) (CA INDEX NAME)



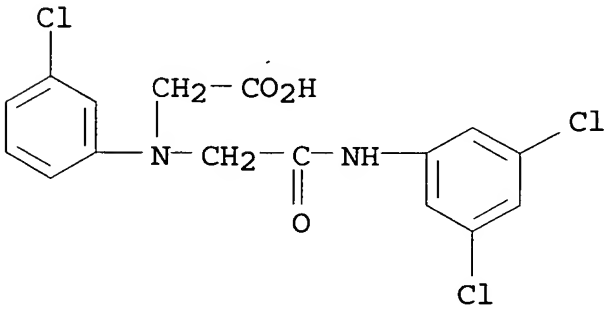
RN 743422-98-2 HCAPLUS
CN Glycine, N-[2-oxo-2-(phenylamino)ethyl]-N-phenyl- (9CI) (CA INDEX NAME)



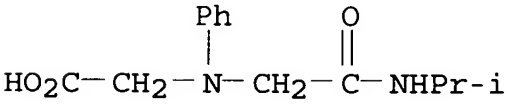
RN 743422-99-3 HCAPLUS
CN Glycine, N-(4-methoxyphenyl)-N-[2-[(4-methoxyphenyl)amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)



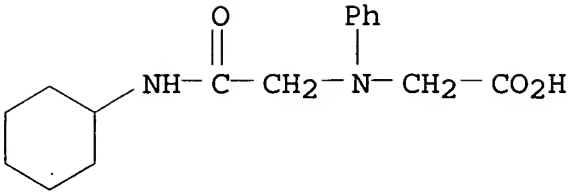
RN 743423-00-9 HCAPLUS
CN Glycine, N-(3-chlorophenyl)-N-[2-[(3,5-dichlorophenyl)amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)



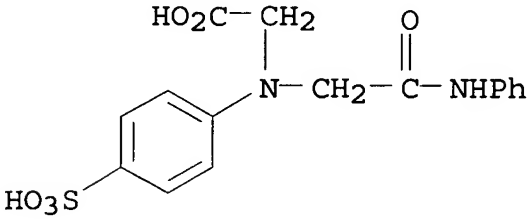
RN 743423-01-0 HCAPLUS
CN Glycine, N-[2-[(1-methylethyl)amino]-2-oxoethyl]-N-phenyl- (9CI) (CA INDEX NAME)



RN 743423-02-1 HCAPLUS
CN Glycine, N-[2-(cyclohexylamino)-2-oxoethyl]-N-phenyl- (9CI) (CA INDEX NAME)



RN 743423-03-2 HCAPLUS
CN Glycine, N-[2-oxo-2-(phenylamino)ethyl]-N-(4-sulfophenyl)- (9CI) (CA INDEX NAME)



IC ICM B41C001-10
ICS G03F007-004
CC 74-6 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
IT 103-01-5 122-59-8 1137-73-1 3959-23-7 6915-15-7
35676-11-0 60085-74-7 62952-26-5 161555-27-7
743422-66-4 743422-67-5 743422-68-6 743422-69-7 743422-70-0
743422-71-1 743422-72-2 **743422-73-3** 743422-74-4
743422-75-5 743422-76-6 743422-77-7 743422-78-8 743422-79-9
743422-80-2 743422-81-3 743422-82-4 743422-83-5 743422-84-6
743422-85-7 743422-86-8 743422-88-0 743422-89-1 743422-90-4
743422-92-6 743422-93-7 743422-96-0 **743422-98-2**
743422-99-3 743423-00-9 743423-01-0
743423-02-1 743423-03-2
RL: TEM (Technical or engineered material use); USES (Uses) (polymerizable composition and lithog. printing plate precursor containing)

L132 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
1997:434343 Document No. 127:103525 Synthesis and antibacterial activity of rare earth(III) complexes with a new amido acid. Shen, Xu; Xie, Yuyuan; Geng, Hongzhi (Dep. Synthetic Chemistry, Shanghai

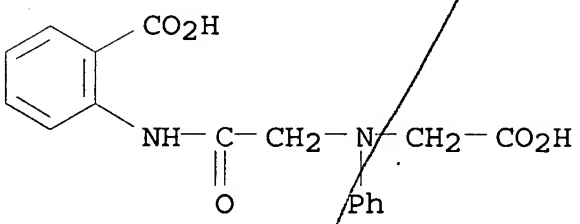
Inst. Materia Medica, Academia Sinica, Shanghai, 200031, Peop. Rep. China). Zhongguo Yaowu Huaxue Zazhi, 5(1), 18-22 (Chinese) 1995. CODEN: ZYHZEF. ISSN: 1005-0108. Publisher: Zhongguo Yaowu Huaxue Zazhi Bianjibu.

AB Ln2L3·4H2O [Ln = La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Yb, Sc, Y; H2L = N-carboxymethyl-N-phenyl-N'-(2-carboxyphenyl)glycine amide] were prepared and characterized by elemental anal., IR, molar conductance, 1H NMR,TG and DTA. Pharmacol. tests indicated that these complexes possessed some inhibiting activity against B. subtilis 6633, S. lutea, S. aureus 209p, P. diplococcus, E. coli and P. aeruginosa x313.

IT **192068-03-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(complexation with rare earth metals and antibacterial activity)

RN 192068-03-4 HCAPLUS

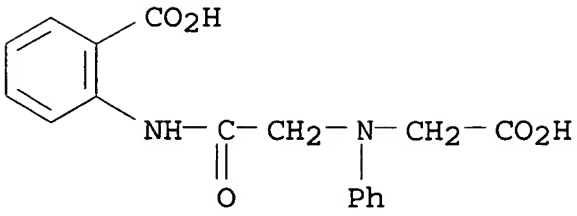
CN Benzoic acid, 2-[[[(carboxymethyl)phenylamino]acetyl]amino]- (9CI) (CA INDEX NAME)



IT **192068-03-4DP**, rare earth complexes
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermal decomposition and antibacterial activity)

RN 192068-03-4 HCAPLUS

CN Benzoic acid, 2-[[[(carboxymethyl)phenylamino]acetyl]amino]- (9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 10

IT **192068-03-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(complexation with rare earth metals and antibacterial activity)

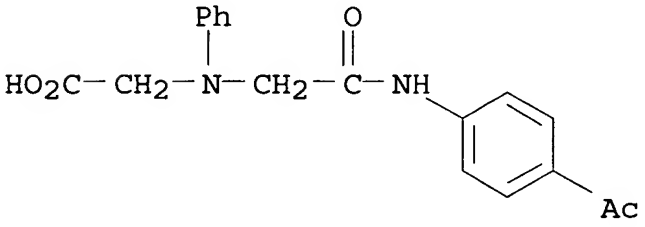
IT 7439-91-0DP, Lanthanum, N-carboxymethyl-N-phenyl-N'-(2-carboxyphenyl)glycine amide, preparation 7440-60-0DP, Holmium, N-carboxymethyl-N-phenyl-N'-(2-carboxyphenyl)glycine amide, preparation **192068-03-4DP**, rare earth complexes
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermal decomposition and antibacterial activity)

L132 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
1995:605967 Document No. 123:73388 Lanthanide (III) complexes with a hydrazone derived from a novel amido acid and isonicotinic acid hydrazide: synthesis, characterization and antibacterial activity. Shen, Xu; Xie, Yuyuan; Jiang, Hualiang (Dep. Synthetic Chem., Shanghai Inst. Materia Medica, Shanghai, 200031, Peop. Rep. China). Synthesis and Reactivity in Inorganic and Metal-Organic Chemistry, 25(4), 511-19 (English) 1995. CODEN: SRIMCN. ISSN: 0094-5714. Publisher: Dekker.

AB LnL3.6H2O (Ln = La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Yb, Y; HL = N-isonicotinamido-4-N-[(N-carboxymethyl-N-phenyl)aminoacetyl]aminoacetophenonaldimine) were synthesized and characterized from elemental analyses, magnetic moment measurements, IR, 1H NMR and UV-visible spectra, molar conductance, TG and DTA. Preliminary pharmacol. tests showed that these complexes possess inhibiting activities against B. subtilis 6633, S. lutea, S. aureus 209p, P. diplococcus, E. coli and P. aeruginosa x313.

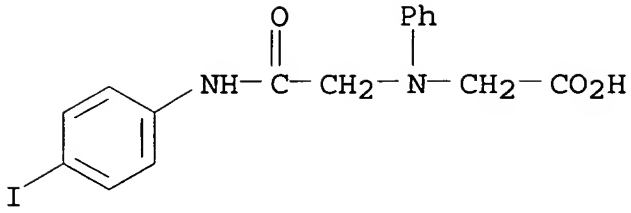
IT **164739-82-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT (Reactant or reagent)
(preparation and reaction with isonicotinic acid hydrazide)
RN 164739-82-6 HCAPLUS
CN Glycine, N-[2-[(4-acetylphenyl)amino]-2-oxoethyl]-N-phenyl- (9CI) (CA INDEX NAME)



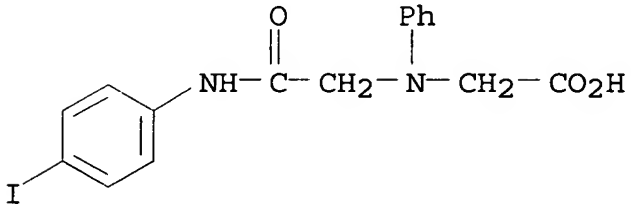
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 10, 27
IT **164739-82-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with isonicotinic acid hydrazide)

L132 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
1995:236994 Document No. 122:70619 Synthesis and characterization of lanthanide(III) chelates with (N-carboxymethyl-N-phenyl-N'-4-iodophenyl)glycinamide. Shen, Xu; Xie, Yuyuan; Geng, Hongzhi (Shanghai Inst. Materia Medica, Acad. Sinica, Shanghai, 200031, Peop. Rep. China). Synthesis and Reactivity in Inorganic and Metal-Organic Chemistry, 24(10), 1745-52 (English) 1994. CODEN: SRIMCN. ISSN: 0094-5714. Publisher: Dekker.
AB Twelve lanthanide complexes [Ln(CPIG)3].6H2O (Ln = La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Yb; HCPIG = N-carboxymethyl-N-phenyl-N'-4-iodophenyl-glycinamide) were synthesized by the reaction of HCPIG with lanthanide chlorides, and characterized by elemental analyses, IR, 1HNMR, DTA, TG and molar conductances. Molar conductances of these complexes in DMF suggest them to be nonelectrolytes.
IT **160293-90-3P 160293-91-4P**, (N-Carboxymethyl-N-phenyl-N'-4-iodophenyl)glycinamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of lanthanide complexes)
RN 160293-90-3 HCAPLUS
CN Glycine, N-[2-[(4-iodophenyl)amino]-2-oxoethyl]-N-phenyl-, monosodium salt (9CI) (CA INDEX NAME)



● Na

RN 160293-91-4 HCAPLUS
CN Glycine, N-[2-[(4-iodophenyl)amino]-2-oxoethyl]-N-phenyl- (9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)
IT **160293-90-3P 160293-91-4P**, (N-Carboxymethyl-N-phenyl-N'-4-iodophenyl)glycinamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of lanthanide complexes)

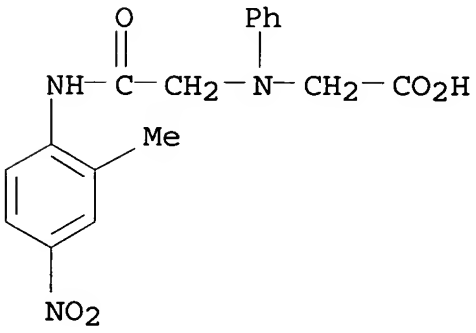
L132 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
1995:111203 Document No. 122:44862 Lanthanide(III) complexes of a new acid amide ligand derived from 2-amino-5-nitrotoluene: synthesis and characterization. Shen, Xu; Xie, Yuyuan; Jiang, Hualiang; Geng, Hongzhi (Dep. Synthetic Chem., Shanghai Inst. Material Medica, Shanghai, 200031, Peop. Rep. China). Polish Journal of Chemistry, 68(9), 1683-8 (English) 1994. CODEN: PJCHDQ. ISSN: 0137-5083.
AB Fourteen complexes Ln(CPGA)3·nH2O (HCPGA = N-carboxymethyl-N-phenyl-N'-[2-methyl-4-nitrophenyl]glycine amide; Ln = La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Yb, Y, n = 6; Ln = Sc, n = 2) were synthesized and characterized from elemental anal.,

IR, molar conductance, 1H NMR, TG and DTA. Molar conductance of the complexes in DMF suggested them to be nonelectrolytes.

IT **159973-69-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with rare earth chlorides)

RN 159973-69-0 HCAPLUS

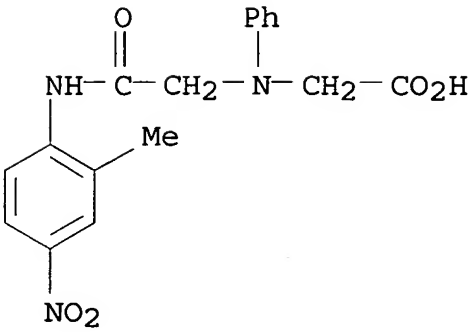
CN Glycine, N-[2-[(2-methyl-4-nitrophenyl)amino]-2-oxoethyl]-N-phenyl- (9CI) (CA INDEX NAME)



IT **159973-54-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 159973-54-3 HCAPLUS

CN Glycine, N-[2-[(2-methyl-4-nitrophenyl)amino]-2-oxoethyl]-N-phenyl-, monosodium salt (9CI) (CA INDEX NAME)



● Na

CC 78-7 (Inorganic Chemicals and Reactions)

IT **159973-69-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with rare earth chlorides)

IT **159973-54-3P** 159973-61-2P 159973-62-3P 159973-63-4P 159973-64-5P 159973-65-6P 159973-66-7P 159973-67-8P 159973-68-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L132 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
1981:438681 Document No. 95:38681 Diaminotriacetic acid and its chelates bound on a substrate. Wieder, Irwin; Wollenberg, Robert H. (Analytical Radiation Corp., USA). Ger. Offen. DE 3033691 19810319, 42 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1980-3033691 19800908.

AB Diaminotriacetic acid-organic compound-metal-activator complexes are described for fluorescence assays, especially fluorescence immunoassays.

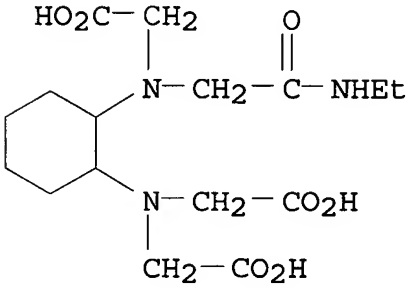
In 1 example, thyroxine was bound to EDTA dianhydride, and the remaining anhydride group was hydrolyzed. The conjugate product, thyroxine-ethylenediaminetriacetic acid, was purified on a silica gel column and by TLC. A complex of Tb and the conjugate was formed. When a ternary complex was formed with 5-sulfosalicylate (as activator), it was used as a label in a fluorescence immunoassay for thyroxine. Examples are also given for preparation of other complexes and for detns. of antibodies, cells, thyronine and

bacteria.

IT **77975-70-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with europium)

RN 77975-70-3 HCAPLUS

CN Glycine, N-[2-[bis(carboxymethyl)amino]cyclohexyl]-N-[2-(ethylamino)-2-oxoethyl]- (9CI) (CA INDEX NAME)



IC C07C103-50; C07J041-00; C07G007-00; C07G017-00

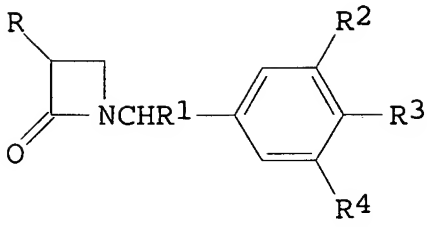
CC 9-6 (Biochemical Methods)
Section cross-reference(s): 2, 15

IT **77975-70-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with europium)

L132 ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN

1981:65461 Document No. 94:65461 4-Unsubstituted azetidinone derivatives. Hashimoto, Masashi; Hemmi, Keiji; Kamiya, Takashi; Komori, Tadaaki; Nakaguti, Osamu; Saito, Yoshihisa; Shiokawa, Youichi; Takasugi, Hisahi; Takaya, Takao; Teraji, Tsutomu (Fujisawa Pharmaceutical Co., Ltd., Japan). U.S. US 4207234 19800610, 130 pp. Cont.-in-part of U.S. Ser. No. 694,891, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1977-858375 19771207.

GI



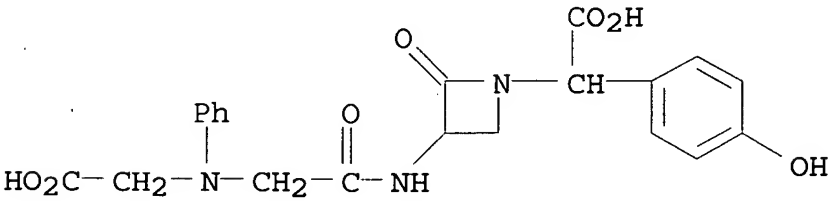
I

AB Lactacillanic acids and analogs I (R = NH2, acylamino, benzenesulfonamido; R1 = CO2H, pharmaceutically acceptable salt or ester derivative of CO2H; R2 = H, NH2, NO2, halo, alkoxy, alkylthio; R3 = H, OH, alkyl, alkylthio, OCH2Ph; R4 = H, Halo, alkoxy, alkylthio), which showed bactericidal activity, were prepared Thus, 3-aminolactacillanic acid reacted with PhCH2COCl in water-Me2CO containing NaHCO3 to yield I (R = PhCH2CONH, R1 = CO2H, R3 = OH, R2 = R4 = H).

IT **75244-76-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 75244-76-7 HCAPLUS

CN 1-Azetidineacetic acid, 3-[[[(carboxymethyl)phenylamino]acetyl]amino]-α-(4-hydroxyphenyl)-2-oxo- (9CI) (CA INDEX NAME)



IC C07D205-08; C07D401-12; C07D403-12; C07D409-12

INCL 260239000A

CC 27-5 (Heterocyclic Compounds (One Hetero Atom))

IT 59511-76-1P 59511-77-2P 59511-78-3P 59511-79-4P 59511-81-8P
59511-82-9P 59511-83-0P 59511-84-1P 59511-86-3P 59511-87-4P
59511-89-6P 59511-90-9P 59511-91-0P 59511-92-1P 59511-93-2P
59511-96-5P 59511-97-6P 59511-99-8P 59512-01-5P 59512-02-6P
59512-03-7P 59547-68-1P 59547-69-2P 59547-70-5P 62105-86-6P

62634-84-8P 64026-60-4P 64026-63-7P 64026-64-8P 64026-68-2P
64026-69-3P 64026-75-1P 64026-77-3P 64026-78-4P 64026-79-5P
64026-80-8P 64026-81-9P 64026-82-0P 64026-84-2P 64026-85-3P
64026-86-4P 64026-88-6P 64026-89-7P 64026-90-0P 64026-91-1P
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64027-05-0P 64027-11-8P 64027-13-0P 64027-15-2P 64027-16-3P
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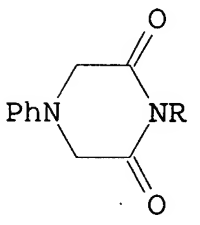
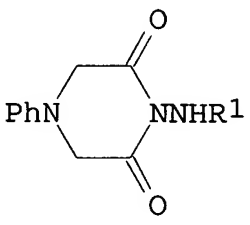
75270-56-3P 75270-57-4P 75283-26-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L132 ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
1977:453210 Document No. 87:53210 Preparation and cyclization of N-carboxymethyl-N-phenylglycylhydrazines. Tanaka, Tatsuo; Komuro, Masakatsu; Ohta, Masaki (Fac. Eng., Ibaraki Univ., Hitachi, Japan). Yuki Gosei Kagaku Kyokaishi, 34(10), 719-21 (Japanese) 1976. CODEN: YGKKAE. ISSN: 0037-9980.

GI



I



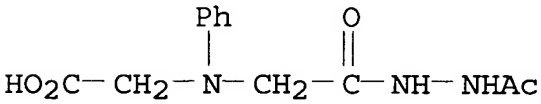
III

AB Reactions of N-phenyliminodiacetic anhydride (I) with a variety of

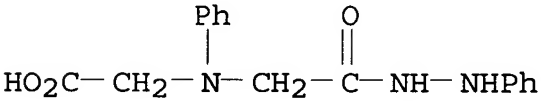
hydrazine derivs. gave N-carboxymethyl-N-phenylglycylhydrazines HO2CCH2NPhCH2CONHNHR (II, R = COCH2NPhCH2CO2H, Ac, Ph, PhCO) in 56-94% yields. Fusion of II under reduced pressure or heating with Ac2O gave the 2,6-piperazinediones III (R1 = 4-phenyl-2,4-dioxo-1-piperazinyl, AcNH, PhNH, Ac2N, AcNPh, PhCONH, BzNAc).

IT **63529-72-6P 63529-73-7P 63529-74-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, phenylpiperazinedione derivs. from)

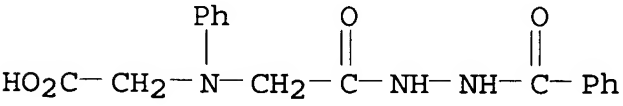
RN 63529-72-6 HCAPLUS
CN Glycine, N-[2-(2-acetylhydrazino)-2-oxoethyl]-N-phenyl- (9CI) (CA INDEX NAME)



RN 63529-73-7 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-phenyl-, 1-(2-phenylhydrazide) (9CI) (CA INDEX NAME)



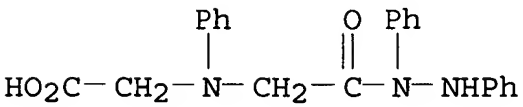
RN 63529-74-8 HCAPLUS
CN Benzoic acid, 2-[[(carboxymethyl)phenylamino]acetyl]hydrazide (9CI) (CA INDEX NAME)



IT **63529-75-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

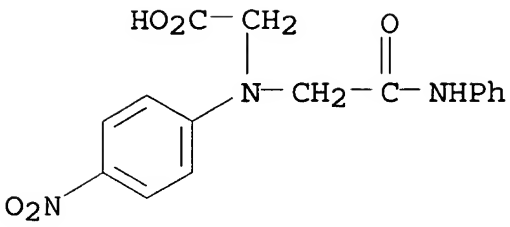
RN 63529-75-9 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-phenyl-, 1-(1,2-diphenylhydrazide)

(9CI) (CA INDEX NAME)

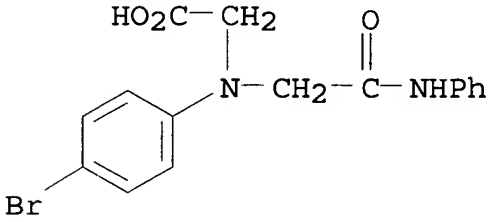


CC 28-18 (Heterocyclic Compounds (More Than One Hetero Atom))
IT 63529-71-5P **63529-72-6P 63529-73-7P**
63529-74-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, phenylpiperazinedione derivs. from)
IT **63529-75-9P** 63529-76-0P 63529-77-1P 63529-78-2P
63529-79-3P 63529-80-6P 63529-81-7P 63529-82-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

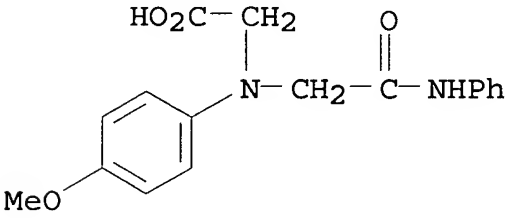
L132 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
1972:113170 Document No. 76:113170 Conjugated systems obtained by reaction of cyclic amides with dehydrogenation and dehydration agents. III. Mesoionic compounds. Anhydro dihydroxides of 1,4-disubstituted-3,5-bis(arylthio)-2,6-dihydroxypyrazinium. Sorm, M.; Honzl, J. (Inst. Macromol. Chem., Czech. Acad. Sci., Prague, Czech.). Tetrahedron, 28(3), 603-10 (English) 1972. CODEN: TETRAB. ISSN: 0040-4020. OTHER SOURCES: CASREACT 76:113170.
GI For diagram(s), see printed CA Issue.
AB Derivs. of anhydro-3,5-bis(phenylthio)-2,6-dihydroxy-1,4-diphenylpyrazinium dihydroxide with H atoms at the para positions of the Ph rings systematically substituted with a NO2 group, Br and a OMe group and derivs. of the same compound with Ph groups systematically substituted with Me groups at positions 1 and 4 were prepared The ir, NMR and electronic spectra of these compds. are in agreement with the assumed prevailing participation of an aromatic canonic structure (I) in their real structure.
IT **35676-09-6P 35676-10-9P 35676-11-0P**
35676-12-1P 35676-13-2P 35676-14-3P
35676-18-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35676-09-6 HCAPLUS
CN Glycine, N-(4-nitrophenyl)-N-[2-oxo-2-(phenylamino)ethyl]- (9CI) (CA INDEX NAME)



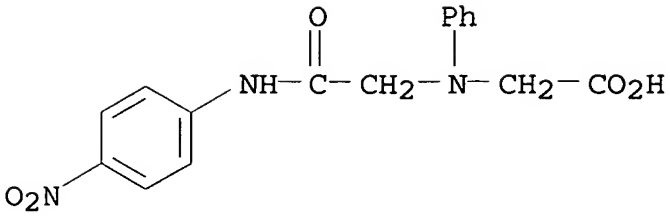
RN 35676-10-9 HCAPLUS
CN Glycine, N-(4-bromophenyl)-N-[2-oxo-2-(phenylamino)ethyl]- (9CI)
(CA INDEX NAME)



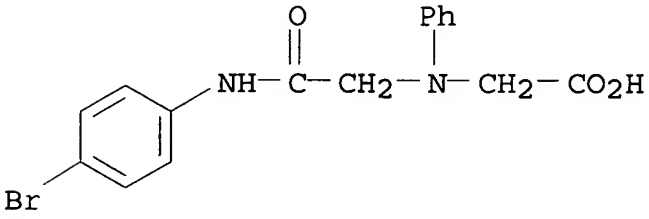
RN 35676-11-0 HCAPLUS
CN Glycine, N-(4-methoxyphenyl)-N-[2-oxo-2-(phenylamino)ethyl]- (9CI)
(CA INDEX NAME)



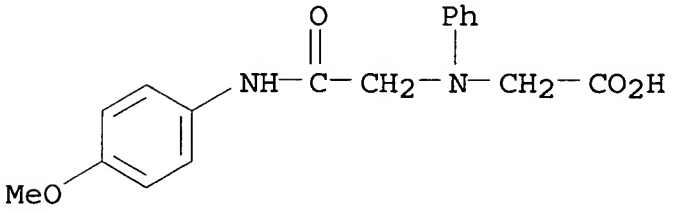
RN 35676-12-1 HCAPLUS
CN Glycine, N-[2-[(4-nitrophenyl)amino]-2-oxoethyl]-N-phenyl- (9CI)
(CA INDEX NAME)



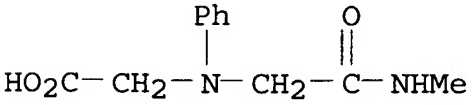
RN 35676-13-2 HCAPLUS
CN Glycine, N-[2-[(4-bromophenyl)amino]-2-oxoethyl]-N-phenyl- (9CI) (CA INDEX NAME)



RN 35676-14-3 HCAPLUS
CN Glycine, N-[2-[(4-methoxyphenyl)amino]-2-oxoethyl]-N-phenyl- (9CI) (CA INDEX NAME)



RN 35676-18-7 HCAPLUS
CN Glycine, N-[2-(methylamino)-2-oxoethyl]-N-phenyl- (9CI) (CA INDEX NAME)



CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))
IT 12694-01-8P 12694-15-4P 12694-16-5P 12694-27-8P 12694-28-9P
12694-29-0P 12694-30-3P 12694-31-4P 12694-32-5P 12694-38-1P
12694-39-2P 12694-42-7P 13480-10-9P 27356-38-3P 30810-75-4P
35676-04-1P 35676-05-2P 35676-06-3P 35676-07-4P 35676-08-5P
35676-09-6P 35676-10-9P 35676-11-0P
35676-12-1P 35676-13-2P 35676-14-3P
35676-15-4P 35676-16-5P 35676-17-6P **35676-18-7P**
35727-40-3P 35727-42-5P 35820-94-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

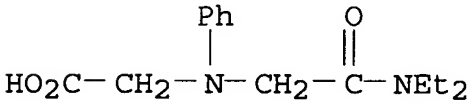
L132 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
1961:27903 Document No. 55:27903 Original Reference No. 55:5503i,5504a-i,5505a-c Aniline derivatives with pharmacologic activity. Larizza, Angelo; Brancaccio, Giovanni (Cutolo-Calois S.A., Naples). Gazzetta Chimica Italiana, 89, 2402-20 (Unavailable) 1959. CODEN: GCITA9. ISSN: 0016-5603.

AB In consideration of the interesting analgesic and local anesthetic properties of PhNHCH2CONEt2 (I) (U.S. 2,568,142, CA 46, 3568a), 52 new derivs., PhNRR' (II), were prepared PhNH2 (or PhNMe) (0.2 mole) and 0.1 mole of a chloro- or bromoacyl amide heated 24 hrs. at 100° and the cooled mass taken up in C6H6, the filtered solution stirred with 10-15% aqueous K2CO3 and the residue on evaporation distilled gave solid or dense oily II, readily forming picrates and HCl salts. PhNH2 (18.6 g.) and 20.8 g. MeCHBrCONEt2 heated 24 hrs. at 100° the cooled mass taken up in 200 ml. C6H6 and filtered from PhNH2.HBr, the washed and dried filtrate evaporated and the residue distilled at 129°/0.3 mm. yielded 80-5% II (R = H, R' = CHMeCONEt2), m. 79-80° (ligroine). I treated with PhCH2Cl gave II (R = PhCH2, R' = CH2CONEt2), m. 75° (ligroine). Data for this group were [R, R', m.p. (uncor.), b.p./mm., nD/temperature, salt and m.p. salt given): H, CONEt2, 84-5°, -, -, -, -; H, CH2CONMe2, 116-17°, 140-1°/0.1, -, HCl salt, 174-5°; H, CH2CONEt2, -, 142°/0.4, 1.5509/24°, picrate, 154-5°; H, CH2CH2CONEt2, -, 142-5°/0.09, 1.5463/24°, picrate, 120-2°; H, CHMeCONEt2, 79-80°, 128-30°/0.3, -, HCl salt, 167-8°; H, CHEtCONEt2, 59-60°, 105-8°/0.01 -, -, -; H, CH2CONHCH2CONEt2, 78-9°, 200°/0.07, -, picrate, 147-8°; H, CH2CONC4H8 (NC4H8-pyrrolidino), 134-5°, 156-8°/0.2, -, picrate, 161-2°; H, CH2CONC5H10

(NC5H10-piperidino), 106-7°, 180-5°/0.08, -, picrate, 154-5°; H, CH2CONC4H8O (NC4H8O-morpholino), 109-10°, 174-7°/0.15, -, picrate, 154-5°; H, CHMeCONC4H8, 110-11°, 170-2°/0.5, -, HCl salt, 174-5°; H, CHMeCONC5H10, 86-8°, 145-50°/0.05, -, HCl salt, 182-4°; H, CHMeCONC4H8O, 149-50°, 170-2°/0.06, -, HCl salt, 192-3°; Me, CH2CONMe2, -, 125-8°/0.1, 1.5658/30°, -, -; Me, CH2CONEt2, -, 136-40°/0.15, 1.5516/18°, HCl salt, 148-5°, MeI salt, 130-1°; Me, CH2CH2CONEt2, -, 139-40°/0.25, 1.5540/20°, MeI, 130-1°; Me, CHMeCONEt2, 45-6°, 115-20°/0.2, -, -, -; Me, CHEtCONEt2 (III), -, 118-22°/0.12, 1.5370/29°, -, -; Me, CH2CONC4H8, 62-3° (ligroine), 150-2°/0.1 -, -, -; Me, CH2CONC5H10, 79-80° (ligroine), 158-60°/0.1, -, MeI salt, 122-4°; Me, CH2CONC4H8O, 110-12° (ligroine), 160-2°/0.15, -, -, -; PhCH2, CH2CONEt2, 75-6° (ligroine), 180-2°/0.05, -, HCl salt, 156-7°. PhNHCH2CONEt2 (0.2 mole) heated 36 hrs. at 85° with 14.9 g. ClCH2CONEt2 and the cooled product extracted with C6H6, the washed (aqueous K2CO3) and dried extract evaporated and the residue distilled in vacuo gave II (R = R' = CH2CONEt2) (IV), m. 123-4° (ligroine) converted to II (R = R' = CH2CH2NEt2) by reduction with LiAlH4. Acidification of the alkaline washings with HCl gave II (R = CH2CO2H, R' = CH2CONEt2). Data for II were (R, R', m.p., b.p./mm., and nD/temperature given): CH2CH2OH, CH2CONEt2, 62-3° (ligroine), 160-70°/0.11, -; CH2CO2H, CH2CONEt2, 148°, -, -; CO2Et, CH2CONEt2, 50-1, 160-2°/0.2, -; CO2Et, CH2CH2CONEt2, -, 155-6°/0.07, 1.5121-24°; CH2CONEt, CH2CONEt (IV), 125-6° (ligroine), 180-90°/0.1, -; EtCO, CH2CONEt2, 82-3° (ligroine), 150-5°/0.06, -; EtCO, CH2CONC5H10, 90-1° (ligroine), 166-8°/0.05, -; EtCO, CH2CONEt2, -, 130-2°/0.07, 1.5187/28°; EtCO, CHMeCONC4H8, 94-6°, 160-2°/0.15, -; EtCO, CHMeCONC5H10, -, 146-8°/0.07, 1.5382/28°; EtCO, CHMeCONC4H8O, 86-7°, 158-60°/0.03, -. PhNMe (10.7 g.) and 14.9 g. MeCHClCH2NEt2 heated 24 hrs. at 100° and the cooled product taken up in H2O, made alkaline with aqueous K2CO3 and extracted with C6H6, the dried (anhydrous K2CO3) extract evaporated in vacuo and the residue distilled yielded 80% II (R = Me, R' = CHMeCH2NEt2), b0.08 78-80°. Data for II were (R, R', m.p., b.p./mm., nD/temperature, and, where given, salts and m.p.): H, CH2CH2NC4H8, -,

93°/0.08, 1.5568/23°; H, CH2CH2NC5H10, -, 97-9°/0.07, 1.5515/24°, picrate, 155-7°; H, CH2CH2NC4H8O, -, 107-10°/0.06, 1.5578/24°, picrate, 180-1°; H, CHMeCH2NC4H8 (V), -, 80-2°/0.05, 1.5188/24°, picrate, 105-6°; H, CHMeCH2NC4H8, -, 112-13°/0.1, 1.5469/24°, picrate, 140-1°; Me, CH2CH2NEt2, -, 95-9°/0.12, 1.5258/25°, picrate, 142-3°; Me, CHMeCH2NEt2, -, 78-80°/0.08, 1.5195/29°, picrate, 136-7°; CH2CONEt2, CH2CH2NEt2, -, 150-5°/0.1, 1.5252/25°, MeI salt, 105-6°; CH2CH2NEt2, CH2CH2NEt2, -, 115-18°/0.1, 1.5108/30°, picrate, 163-5°. PhNHCH2CH2NEt2 (192 g.) and 14.0 BzCl heated 24 hrs. at 100° and the mixture taken up in H2O, made alkaline with K2CO3 and extracted with C6H6, the dried extract evaporated and the residue distilled in vacuo yielded 80-5% II (R = Bz, R' = CH2CH2NEt2). Other II were (R, R', b.p./mm., nD/temperature, and, where given, salt and m.p. salt): Ac, CH2CH2NEt2, 98-100°/0.07, 1.5068/29°; COEt, CH2CH2NEt2, 104-6/0.1, 1.5054/29°; Bz, CH2CH2NEt2, 146-8°/0.25, 1.5598/24°, picrate, 121-2°; CO2Et, CH2CH2NH2, 101-3°/0.2, 1.4983/28°, picrate, 78-9°; CO2Et, (CH2)3NEt2, 123-5°/0.07, -; CH2CH2OH, CH2CH2NEt2, 130-5°/0.09, 1.5369/24°, picrate, 116-17°; Ac, CH2CH2NC4H8, 119-21°/0.5, 1.5262/24°; COEt, CH2CH2NC4H8, 119-22°/0.04, 1.5242/24°; Bz, CH2CH2NC4H8 [m. 130-2° (ligroine)], 150-5°/0.06, -, picrate, 166-8°; Ac, CH2CH2NC5H10, 122-5°/0.3, 1.5294/24°; COEt, CH2CH2NC5H10, 125-7°/0.09, 1.5242/24°, picrate, 132-3°; Bz, CH2CH2NC5H10, 158-60°/0.18, 1.5720/24°, picrate, 202-3°; Ac, CH2CH2NC4H8O, 126-8°/0.16, 1.5235/24°, HCl salt, 182-3°, picrate, 142-3°; COEt, CH2CH2NC4H8O, 130-3°/0.06, 1.5245/24°, picrate, 132-3°; Bz, CH2CH2NC4H8O, 180-2°/0.12, 1.5765/24°, picrate, 209-11°; Ac, CHMeCH2NEt2, 103-5°/0.08, 1.5048/29°, picrate, 128-9°; COEt, CHMeCH2NEt2, 110-12°/0.12, 1.5046/24°, picrate, 109-11°; Bz, CHMeCH2NEt2, 145-8°/0.12, 1.5510/24°, picrate, 110-11°; Ac, CHMeCH2NC4H8, 120-4°/0.2, 1.5245/24°, picrate, 144-5°; COEt, CHMeCH2NC4H8, 116-18°/0.06, 1.5228/24°, HCl salt, 179-80°; Bz, CHMeCH2NC4H8 (VI), 148-50°/0.06, 1.5688/24°, picrate, 120-2°. The infrared spectra of compds. III-VI were reported and presented maximum conformity.

IT **100876-32-2**, Glycine, N-(diethylcarbamoylmethyl)-N-phenyl-
(preparation of)
RN 100876-32-2 HCAPLUS
CN Glycine, N-(diethylcarbamoylmethyl)-N-phenyl- (6CI) (CA INDEX NAME)



CC 10G (Organic Chemistry: Heterocyclic Compounds)
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101260-54-2, Acetanilide, N-(2-diethylamino-1-methylethyl)-
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Morpholine, 4-(N-phenylsarcosyl)- 101353-63-3, Acetanilide,
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Diethylenetriamine, 1,1,7,7-tetraethyl-4-phenyl-, dipicrate 130862-40-7, Acetanilide, N-(2-diethylaminoethyl)- 131253-11-7, Butyramide, N,N-diethyl-2-N-methylanilino- 131732-89-3, Morpholine, 4-N-phenylalanyl-, hydrochloride 132569-93-8, Ammonium, dimethylphenyl(piperidinocarbonylmethyl)-, iodide 859919-70-3, Carbanilic acid, N-(2-diethylaminoethyl)-, picrate (preparation of)

L132 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
1921:18605 Document No. 15:18605 Original Reference No. 15:3465g-i,3466a-i,3467a-i,3468a Acetic acid derivatives of p-anisidine. Halberkann, J. (Inst. Schiffs-u. Tropenkrankheiten, Hamburg, Germany). Ber., 54B, 1152-67 (Unavailable) 1921.
AB 4-Methoxyphenylaminoacetic acid (N-p-anisylglycine) (A), from 20 g. p-anisidine (B), 33 g. NaOAc and 4 cc. H2O heated 0.5 hr. on the H2O bath with 14.5 g. ClCH2CO2H, treated with excess of KOH, freed from B with Et2O, strongly acidified with HCl, freed from the tertiary amine by repeated extraction with Et2O and neutralized to Congo with KOH,
stout needles from AcOEt-benzine, slender tablets from H2O, m. 154-7° (decomposition), has a fatty feeling, more or less quickly turns yellow to brown in solution and in the light and on heating to 100°, easily, soluble in AcOH (first with a brownish, then a violet color), dilute acids and alkalies, in H2O with a strong acid reaction, Br turning the soln, blue-violet with strong blue fluorescence changed by NH4OH to green, gives with FeCl3 a blue-violet color changing to violet-red, reduces AgNO3 with faint mirror formation, the liquid becoming blue-violet, reduces KMnO4 with formation of a red solution, gives white ppts. with HgNO3 and Hg(NO3)2 which dissolve on heating but reduction follows almost immediately and the solution becomes blue-violet to red. HgCl2 after long standing produces a yellow crystalline precipitate, with slow reduction.
Triketohydrindene gives no color. Alkaline Br solution added to A in H2O
produces a play of colors from yellow through green, brown-red, brown to dark brown-red; if a drop of PhOH has previously been added it changes on the addition of the NaOBr quickly through green and brownish yellow to blue and after long standing, to violet and finally red. Aqueous solns. give no color with Co and Ni salts but with
a trace of CuSO4 become intensely green, NH4OH changing the solution through pink to violet and finally deep violet-blue. Copper salt, obtained by boiling solns. of A with CuCO3, dull dark green powder of very fine yellow-green needles. Zinc salt, stout prismatic

needles. Acetyl derivative (C), from A heated some time with 2 mols. Ac2O, stout whetstone-like needles from alc., m. 185°, easily soluble in alkalies, insol. in dilute acids, gives no color with FeCl3, Br water and NaOBr with or without PhOH, does not reduce Ag, Hg' or Hg'' nitrate, does not change the color of CuSO4 solution Ethyl ester, from 20 g. B, 10 g. ClCH2CO2Et and 20 g. AcOEt heated 5 hrs. on the H2O bath, stout prisms from H2O, long rectangular plates from alc., thick table-like prisms from ligroin, m. 57-8°, easily soluble in dilute acids, gradually resinifies even over H2SO4, gives in H2O with FeCl3 a red to blue-violet color, behaves like A towards, Hg', Hg'' and Ag nitrate and NaOBr; with the latter in the presence of PhOH the solution becomes only brown-red, not blue; Br water produces only a faint violet color changed to brownish by NH4OH; CuSO4 solution is not changed in color; acetyl derivative, stable oil easily soluble in the usual organic solvents, gives no color with FeCl3.

Amide, from the ester and alc. NH3 at 100°, needles from petr. ether, cholesterol-like tablets or needles from dilute alc., m. 146-7°, easily soluble in dilute acids, gives in aqueous alc. with FeCl3 a violet-red color. Chloroaceto-4-methoxyphenylamide (D), from 20 g. B in 150 cc. cold dry C6H6 treated dropwise with 9.2 g. ClCH2COCl and 50 cc. C6H6, rectangular leaflets from dilute alc., long needles gradually changing to rhombic needles from absolute alc., m. 121°, gives no color in aqueous alc. with FeCl3, produces itching and sneezing. Triglycolamidic tris-4-methoxyphenylamide, (MeOC6H4NHCOCH2)3N, from D heated 3 hrs, on the H2O bath with 5 parts NH4OH, rectangular tablets from alc., m. 295°, insol. in dilute acids and alkalies, gives in alc. with FeCl3 a red color destroyed by H2O; the alc. mother liquors, treated with H2O until turbid, yield the diglycolamidic bisamide, leaves from H2O, m. 141°, gives a red color with FeCl3, in alc. and with CuSO4 a green color changed to blue by NaOH. 4-Methoxyphenylaminoacet-4-methoxyanilide, from equimol. amts. of B and A heated 2 hrs. at 135°, rectangular leaves from C6H or H2O, m. 134°, long flat needles from alc., gives in alc. with FeCl4 after dilution with H2O a blue-violet, then dirty violet-red color and a violet-blue fluorescence; Br water or vapors color the substance in aqueous suspension green-blue and on heating it dissolves with pink color; in H2SO4 (d. 1.48) it gives a deep red color with FeCl3. The same compound is obtained by heating D and 2 mols. B 2 hrs. at 120° and finally a short time at 140°; acetyl derivative, MeOC6H4NAcCH2CONHC6H4OMe, from equiniol. amts. of B and

C heated about 1 hr. at 175-80°, fine flat needles from 50% alc. or CHCl3-benzine, m. 138°, insol. in dilute acids and alkalies, gives no color with FeCl2. 4-Methoxyphenylbis-4-methoxyphenylaminoacetylamine, (MeOC6H4NHCH2CO)2NC6H4OMe, is formed together with the amide on fusing the components together and remains in the C6H6 mother liquor from which, on concentration and addition of a little benzine, it seps. in rhombic leaflets, m. 185°, difficultly soluble in dilute acids, insol. in alkalies, gives in alc. with FeCl3 an olive-brown color changed by H2O to violet-red (violet-blue in incident light) and in H2SO4 a deep red color. With excess of alc. NaOEt (3 mols.) in the cold D is completely hydrolyzed in 2 days: with 2 mols. NaOEt the chief reaction is the condensation of 2 mols. D to 1,4-bis-4-methoxyphenyl-2,5-diketo-1,4'-diazine hexahydride (E), rhombic leaflets from alc., m. 256°, short needles from (CH2Br)2, better prepared by heating A for 1 hr. at 155-60° in a current of. N. N-4-Methoxyphenyl-N-[4'-methoxyphenylaminoacetyl]aminoacetic acid, from 5 g. E boiled 3 hrs. with 150 cc. alc. and 15.4 cc. of N KOH, freed from most of the alc. by distillation and from the rest by adding 50 cc. H2O and evaporating, treated with 15.4 cc. of N HCl and taken up in Et2O, stout or elongated 6-cornered prisms from 60% alc., sinters 110°, loses H2O, m. turbid 128°, resolidifies and m. again 256°, gives in aqueous alc. with FeCl3 a violet color changing to violet-red or red, soluble without color in H2SO4; solns. in all organic solvents quickly become brown to red: E is easily regenerated, being formed quant. on boiling the C6H6 solution; FeCl3 in H2SO4 produces a red color. 4-Methoxyphenylaminoacetomethyl-4'-methoxyphenylamide (F) is obtained in 3 ways: (1) The alc. mother liquor obtained in the preparation of E by heating A is shaken some time, after suitably concentrating, with soda and the undissolved portion with dilute HCl; the latter extract forms with NaOH a turbidity which is cleared by Et2O and the Et2O extract on evaporation and suitable purification yields a small amount of stout prismatic columns from alc., m. 118°, easily soluble in dilute acids, insol. in alkalies, easily soluble in H2SO4 without color, gives in aqueous alc. with FeCl3 a red color quickly changing to blue-violet and gradually to violet-red, in H2SO4 (d. 1.84) a deep red color. (2) Equimol. amts. of A and p-MeOC6H4NHMe are heated 3 hrs. at 145-50° and the F is extracted from the product (which consists chiefly of E) with alc. (3) F is obtained in good yield by

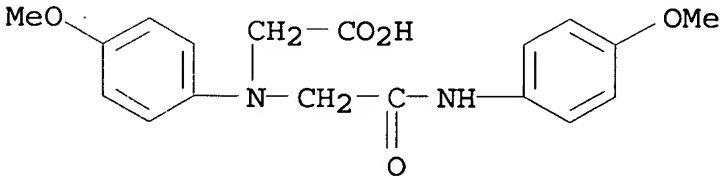
heating chloroacetomethyl-4-methoxyphenylamide 1 hr. at 115° with 2 mols. B. The Cl compound itself is prepared from ClCH2COCl and 2 mols. MeOC6H4NHMe and seps. from C6H6-petr. ether in stout tables, m. 57°, gives no color with FeCl3. N-4-Methoxyphenyldiglycolamidic acid (G) is formed together with A and goes into the Et2O extract of the strongly acidified solution This extract is shaken with acidified H2O and then with dilute KOH, with HCl it yields the G, stout rectangular columns with 1 H2O, gradually deliquesces, assuming a pink color, sinters 89°, m. 95-6° with loss of H2O and m. (anhydrous) 122-3° (decomposition); the solution in AcOH slowly becomes blue, then violet, that in CHCl3 red, those in other organic solvents brownish, that in H2O Violet; a concentrated solution gives with FeCl3 a red color changing on dilution through red-violet and violet-blue back to red-violet; Br vapors produce a green to blue fluorescence, the latter being changed back to green by NH4OH; hot AgNO3, and cold CuSO4 behave in the same way as with A; an aqueous solution containing PhOH is gradually colored only a very faint greenish blue by NaOBr; triketohydrindene produces a yellow color in the hot or cold aqueous solution N-4-Methoxyphenyldiglycolamidic bis-4'-methoxyphenylanilide, from G and 2 mols. B heated some time at 170°, very slender, felted, apparently quadrangular needles from C6H6, m. 184-5°, gives no color with FeCl3, soluble without color in H2SO4: a trace of H2O2 or FeCl3 produces a pink color changed by more to a deep greenish blue and on heating through blue and brown to deep red and finally olive-brown. The HCl extract obtained in the purification of the above compound yields on addition of NaOH and extraction with Et2O [methyl-4-methoxyphenyl]aminoaceto-4'-methoxyphenylanilide, long quadrangular needles, m. 129-30°, easily soluble in dilute acids, insol. in alkalies, gives in aqueous alc. with FeCl3 a crimson color, dissolves in H2SO4 (d. 1.84) without color, H2O2 producing a green color changed by more of the oxidizing agent into a violet-red to deep blue and, on heating, through violet-blue and red to olive-brown. This compound is also formed in small amount by heating A and 0.5 mol. D at 130.°. N-4-Methoxyphenyldiglycolamidic 4'-methoxyanilide, MeOC6H4N(CH2CO2H)CH2CONHC6H4OMe, from 2 mols. A and 1 mol. D heated 1 hr. in an indifferent gas at 130°, then

a short time at 140°, tables from 70% alc., sinters 140°, m. 147° (decomposition), easily soluble in alkalies, insol. in dilute acids; the AcOH solution soon becomes deep blue; FeCl3, in aqueous alc. gives a violet-red color, violet-blue in incident light; H2O2 colors the H2SO4 solution through pink and deep green to olive-brown while FeCl3 gives a permanent deep blue color changing on heating through red into olive-brown. The compound is also formed in small amount from B and 0.5 mol. G at 170°; if the fusion is effected at 120° this becomes the main reaction; boiled 2 hrs. with 4 parts Ac2O it gives 1,4-bis-4'-methoxyphenyl-3,5-diketo-1,4-diazine hexahydride, broad table-like needles on slow, long quadrangular needles on rapid cooling from alc., m. 152°, insol. in alkalies and dilute acids, gives no color with FeCl3, easily soluble in H2SO4 (d. 1.84) with orange-yellow color changed by small amts. of an oxidizing agent (H2O2) to a permanent deep red, by larger amts. (FeCl3) through red, red-brown and olive-brown to green.

IT **743422-99-3**, Glycine, N-p-anisyl-N-[(p-anisylcarbamyl)methyl]-
(preparation of)

RN 743422-99-3 HCAPLUS

CN Glycine, N-(4-methoxyphenyl)-N-[2-[(4-methoxyphenyl)amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)



CC 10 (Organic Chemistry)

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(preparation of)

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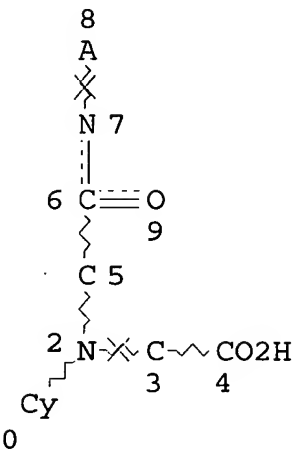


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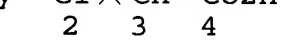


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L133 ANSWER 1 OF 1 CAOLD COPYRIGHT 2005 ACS on STN
AN CA55:5503i CAOLD
TI aniline derivs. with pharmacol. activity
AU Larizza, Angelo; Brancaccio, G.
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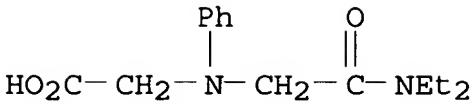

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SEARCH REQUEST FORM

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Requester's Full Name: Sin J. Lee Examiner #: 76060 Date: 9-6-2005
Art Unit: 1752 Phone Number 30X 2-4333 Serial Number: 10/781,862
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If more than one search is submitted, please prioritize searches in order of need.

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Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Plz. Ale B:b.

SCIENTIFIC REFERENCE BR
Sci & Tech Inf Ctr
SEP RECD
Pat. & T.M. Office

Inventors (please provide full names):

Earliest Priority Filing Date:

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Please search for a compound of Cl. #5

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STAFF USE ONLY	Type of Search		Vendors and cost where applicable	
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Searcher Phone #:	AA Sequence (#)		Dialog	
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Online Time: 230	Other		Other (specify)	

PTO-1590 (8-01)

AMENDMENTS TO THE CLAIMS

This listing of claims will replace all prior versions and listings of claims in the application:

LISTING OF CLAIMS:

1. (currently amended): A polymerizable composition comprising:

(A) a compound which causes at least one of decarboxylation and dehydration by heat;

(B) a radical initiator;

(C) a compound having at least one ethylenically unsaturated bond; and

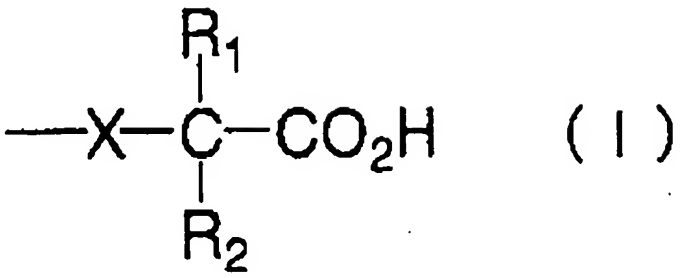
(D) an infrared ray absorber,

wherein the compound (A) and the radical initiator (B) are separate and distinct compounds from each other.

2. (original): The polymerizable composition according to claim 1, wherein the compound (A) is one which causes at least one of decarboxylation and dehydration at a temperature of 100°C to 300°C.

3. (original): The polymerizable composition according to claim 1, wherein the compound (A) is one having a structure capable of forming a 4 to 6-membered lactone ring, a 4 to 6-membered lactam ring or a 4 to 6-membered cyclic acid anhydride.

4. (original): The polymerizable composition according to claim 1, wherein the compound (A) is one having at least one group represented by the following formula (I):



(1)

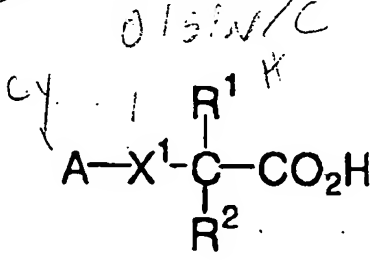
wherein:

X represents a divalent connection group selected from -O-, -S-, -SO_2-, -NH-, -N(R^3)-, and -CO-,

R^3 represents a hydrogen atom or a monovalent substituent,

R^1 and R^2 each independently represents a hydrogen atom or a monovalent substituent, provided that R^1 and R^2, or either one of R^1 and R^2 and R^3 may be taken together to form a ring structure.

5. (original): The polymerizable composition according to claim 1, wherein the compound (A) is a monocarboxylic acid compound represented by the following formula (I-2):



(I-2)

wherein

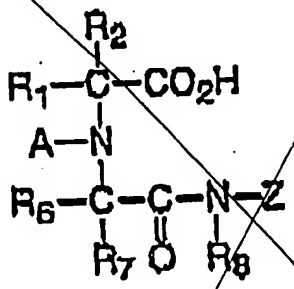
A represents an aromatic group or a heterocyclic group,

R^1 and R^2 each independently represents a hydrogen atom or a monovalent substituent, provided that R^1 and R^2, either one of R^1 and R^2 and X^1, either one of R^1 and R^2 and A, or A and X^1 may be taken together to form a ring structure,

X^1 represents a divalent connection group selected from -O-, -S-, $-SO_2-$, -NH-, $-N(R^3)-$, $-CH_2-$, $-CH(R^4)-$, and $-C(R^4)(R^5)-$, and

R^3, R^4, and R^5 each independently represents a hydrogen atom or a monovalent substituent.

6. (original): The polymerizable composition according to claim 1, wherein the compound (A) is a compound represented by the following formula:



wherein

A represents an aromatic group or a heterocyclic group,

R^1, R^2, R^6, R^7 and R^8 each independently represents a hydrogen atom or a monovalent substituent, provided that R^1 and R^2, either one of R^1 and R^2 and A, or R^8 and Z may be taken together to form a ring structure,

and

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                D ALL
                SEL L1 RN

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                122-59-8/BI OR 161555-27-7/BI OR 35676-11-0/BI OR
                3959-23-7/BI OR 60085-74-7/BI OR 62952-26-5/BI OR
                6915-15-7/BI OR 743422-66-4/BI OR 743422-67-5/BI OR
                743422-68-6/BI OR 743422-69-7/BI OR 743422-70-0/BI OR
                743422-71-1/BI OR 743422-72-2/BI OR 743422-73-3/BI OR
                743422-74-4/BI OR 743422-75-5/BI OR 743422-76-6/BI OR
                743422-77-7/BI OR 743422-78-8/BI OR 743422-79-9/BI OR
                743422-80-2/BI OR 743422-81-3/BI OR 743422-82-4/BI OR
                743422-83-5/BI OR 743422-84-6/BI OR 743422-85-7/BI OR
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                743423-00-9/BI OR 743423-01-0/BI OR 743423-02-1/BI OR
                743423-03-2/BI)
                D SCAN

     FILE 'LREGISTRY' ENTERED AT 08:53:28 ON 22 SEP 2005
L3              STR

     FILE 'REGISTRY' ENTERED AT 09:00:25 ON 22 SEP 2005
L4          50 SEA SSS SAM L3

     FILE 'LREGISTRY' ENTERED AT 09:01:22 ON 22 SEP 2005
L5              STR L3

     FILE 'REGISTRY' ENTERED AT 09:02:41 ON 22 SEP 2005
                D SCAN L2

     FILE 'LREGISTRY' ENTERED AT 09:06:54 ON 22 SEP 2005
L6              STR L5

     FILE 'REGISTRY' ENTERED AT 09:19:04 ON 22 SEP 2005
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L8              STR L6

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L10           1 SEA SSS SAM L8
                D SCAN
L11             SCR 1918
L12          50 SEA SSS SAM L7 NOT L11
                D SCAN L10
L13             SCR 1841
L14          50 SEA SSS SAM L7 NOT L13
L15             SCR 1918 OR 1841
L16          50 SEA SSS SAM L7 NOT L15
L17             SCR 1312
L18          50 SEA SSS SAM L7 AND L17
L19          50 SEA SSS SAM L7 AND L17 NOT L13
L20          50 SEA SSS SAM L7 AND L17 NOT L15
L21             SCR 1312 OR 2036 OR 2021
L22             SCR 1841 OR 2016 OR 1964 OR 1921 OR 1957 OR 1931 OR 1919
L23          50 SEA SSS SAM L7 AND L21 NOT L22
                D QUE STAT
                D QUE STAT L10

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L27          50 SEA SSS SAM L24 AND L21 NOT L26
                D QUE STAT
L28             SCR 1312 AND 1838
L29          50 SEA SSS SAM L24 AND L28
L30          50 SEA SSS SAM L24 AND L28 NOT L26
L31          50 SEA SSS SAM L24 AND L28 NOT L22
                D QUE STAT L31
                D QUE STAT L30
L32             SCR 1526 AND 1838
L33          50 SEA SSS SAM L24 AND L32
L34          50 SEA SSS SAM L24 AND L32 NOT L22
L35          50 SEA SSS SAM L24 AND L32 NOT L26
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L39           50 SEA SSS SAM L36 AND L32 NOT L38
                 D QUE STAT
                 D SAV
L40              SCR 1841 OR 2016 OR 1964 OR 1921 OR 1957 OR 1931 OR 1919
L41           50 SEA SSS SAM L36 AND L32 NOT L40
                 D QUE STAT L39
                 D QUE STAT
                 D QUE L40
                 D QUE L38
L42              SCR 2040
L43           50 SEA SSS SAM L36 AND L32 NOT (L42 OR L38)
L44              SCR 2077
L45           50 SEA SSS SAM L36 AND L32 NOT (L42 OR L38 OR L44)
L46       145388 SEA SSS FUL L36 AND L32 NOT (L42 OR L38 OR L44)
                 D SAV
                 DEL GAR005/A
                 DEL SHO144B/A
                 D SAV
                 SAV TEMP L46 LEE862/A

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     FILE 'HCAPLUS' ENTERED AT 11:24:38 ON 22 SEP 2005
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L49         2743 SEA ABB=ON  PLU=ON  L47
L50        36476 SEA ABB=ON  PLU=ON  DECARBOXYLAT?
L51         4455 SEA ABB=ON  PLU=ON  L48 AND L50
L52              QUE ABB=ON  PLU=ON  POLYMERIZ? OR POLYMERIS? OR POLYM#
                 OR CURE# OR CURING# OR DIGEST? OR CROSSLINK? OR CROSS(W)L
                 INK? OR VULCANIZ? OR VITRIF? OR GEL?
L53          211 SEA ABB=ON  PLU=ON  L51 AND L52
L54       516279 SEA ABB=ON  PLU=ON  POLYMERIZ?
L55          111 SEA ABB=ON  PLU=ON  L54 AND L53
L56         6926 SEA ABB=ON  PLU=ON  (INFRARED OR IR)(2A)ABSORB?
L57            2 SEA ABB=ON  PLU=ON  L56 AND L55
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                D SCAN
L58             3 SEA ABB=ON  PLU=ON  L56 AND L51
L59             3 SEA ABB=ON  PLU=ON  L57 OR L58
L60            52 SEA ABB=ON  PLU=ON  L48 AND L56
L61        656336 SEA ABB=ON  PLU=ON  INFRARED OR IR
L62            11 SEA ABB=ON  PLU=ON  L61 AND L55
L63            19 SEA ABB=ON  PLU=ON  L61 AND L53
L64            52 SEA ABB=ON  PLU=ON  L56 AND L48
L65           159 SEA ABB=ON  PLU=ON  L61 AND L51
                D QUE L52
L66         19758 SEA ABB=ON  PLU=ON  RADICAL(2A)INIT?
L67            12 SEA ABB=ON  PLU=ON  L66 AND L51
L68             5 SEA ABB=ON  PLU=ON  L66 AND L55
L69             1 SEA ABB=ON  PLU=ON  L66 AND L59
                D SCAN
L70        470272 SEA ABB=ON  PLU=ON  74/SC,SX
L71             9 SEA ABB=ON  PLU=ON  L70 AND L55
L72            13 SEA ABB=ON  PLU=ON  L70 AND L53
L73            17 SEA ABB=ON  PLU=ON  L59 OR L68 OR L69 OR L71 OR L72
L74            26 SEA ABB=ON  PLU=ON  L73 OR L62
L75            34 SEA ABB=ON  PLU=ON  L74 OR L63
L76             1 S L75 AND L1
L77            65 S L49 AND L50
L78            62 S L77 NOT L75
L79             7 S L77 AND L52
L80             1 S L79 AND L56
L81             1 S L77 AND L56
L82             3 S L77 AND L66
L83             7 S L77 AND L70
L84            12 S L79-L83
L85            43 S L75 OR L84
L86            31 S L85 NOT L84
L87        137411 S DEHYDRAT? OR DE()HYDRAT?
L88          2911 S L87 AND L48
L89           279 S L88 AND L50
L90            17 S L89 AND L52
L91             1 S L89 AND L56
L92            16 S L89 AND L61
L93             1 S L89 AND L66
L94             2 S L89 AND L70
L95            31 S L90-L94
L96            70 S L95 OR L85
L97           279 S L88 AND L50
L98            17 S L97 AND L52
L99             1 S L98 AND L56
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L100          1 S L98 AND L66
L101          1 S L98 AND L70
L102          1 S L97 AND L56
L103          1 S L97 AND L66
L104          2 S L97 AND L70
L105      19455 S L48 AND L52
L106         27 S L105 AND L56
L107          6 S L106 AND L66
L108         23 S L106 AND L70
L109         16 S L49 AND L56
L110          3 S L109 AND L66
L111         14 S L109 AND L70
L112          9 S L89 AND L54
L113          9 S L95 AND L54
L114         47 S L98-L104 OR L106-L113
L115         30 S L114 AND L54
L116         71 S L115 OR L85
L117         10 S L112 OR L100-L104
L118         15 S L117 OR L107 OR L110 OR L113
L119         57 S L118 OR L85
L120         68 S L119 OR L111
L121         35 S L49 AND L87
L122          5 S L121 AND L52
L123          1 S L121 AND L54
L124          1 S L121 AND L56
L125          1 S L121 AND L66
L126          2 S L121 AND L70
L127          5 S L122-L126
L128         60 S L127 OR L119
L129         71 S L128 OR L120

=> d que stat l128
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                1137-73-1/BI OR 122-59-8/BI OR 161555-27-7/BI OR
                35676-11-0/BI OR 3959-23-7/BI OR 60085-74-7/BI OR
                62952-26-5/BI OR 6915-15-7/BI OR 743422-66-4/BI OR
                743422-67-5/BI OR 743422-68-6/BI OR 743422-69-7/BI OR
                743422-70-0/BI OR 743422-71-1/BI OR 743422-72-2/BI OR
                743422-73-3/BI OR 743422-74-4/BI OR 743422-75-5/BI OR
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                743422-82-4/BI OR 743422-83-5/BI OR 743422-84-6/BI OR
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                743422-93-7/BI OR 743422-96-0/BI OR 743422-98-2/BI OR
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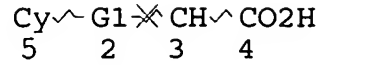
743422-99-3/BI OR 743423-00-9/BI OR 743423-01-0/BI OR
743423-02-1/BI OR 743423-03-2/BI)
L32 SCR 1526 AND 1838
L36 STR



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DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M4-X14 C AT 5

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 4

STEREO ATTRIBUTES: NONE

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L42		SCR 2040
L44		SCR 2077
L46	145388	SEA FILE=REGISTRY SSS FUL L36 AND L32 NOT (L42 OR L38 OR L44)
L47	37	SEA FILE=REGISTRY ABB=ON PLU=ON L2 AND L46
L48	285971	SEA FILE=HCAPLUS ABB=ON PLU=ON L46
L49	2743	SEA FILE=HCAPLUS ABB=ON PLU=ON L47
L50	36476	SEA FILE=HCAPLUS ABB=ON PLU=ON DECARBOXYLAT?
L51	4455	SEA FILE=HCAPLUS ABB=ON PLU=ON L48 AND L50
L52		QUE ABB=ON PLU=ON POLYMERIZ? OR POLYMERIS? OR POLYM# OR CURE# OR CURING# OR DIGEST? OR CROSSLINK? OR CROSS(W)LINK? OR VULCANIZ? OR VITRIF? OR GEL?
L53	211	SEA FILE=HCAPLUS ABB=ON PLU=ON L51 AND L52
L54	516279	SEA FILE=HCAPLUS ABB=ON PLU=ON POLYMERIZ?
L55	111	SEA FILE=HCAPLUS ABB=ON PLU=ON L54 AND L53
L56	6926	SEA FILE=HCAPLUS ABB=ON PLU=ON (INFRARED OR IR)(2A)ABSORB?
L57	2	SEA FILE=HCAPLUS ABB=ON PLU=ON L56 AND L55
L58	3	SEA FILE=HCAPLUS ABB=ON PLU=ON L56 AND L51
L59	3	SEA FILE=HCAPLUS ABB=ON PLU=ON L57 OR L58
L61	656336	SEA FILE=HCAPLUS ABB=ON PLU=ON INFRARED OR IR
L62	11	SEA FILE=HCAPLUS ABB=ON PLU=ON L61 AND L55
L63	19	SEA FILE=HCAPLUS ABB=ON PLU=ON L61 AND L53
L66	19758	SEA FILE=HCAPLUS ABB=ON PLU=ON RADICAL(2A)INIT?

L68	5	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L66 AND L55
L69	1	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L66 AND L59
L70	470272	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON 74/SC,SX
L71	9	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L70 AND L55
L72	13	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L70 AND L53
L73	17	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L59 OR L68 OR L69 OR L71 OR L72
L74	26	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L73 OR L62
L75	34	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L74 OR L63
L77	65	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L49 AND L50
L79	7	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L77 AND L52
L80	1	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L79 AND L56
L81	1	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L77 AND L56
L82	3	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L77 AND L66
L83	7	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L77 AND L70
L84	12	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON (L79 OR L80 OR L81 OR L82 OR L83)
L85	43	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L75 OR L84
L87	137411	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON DEHYDRAT? OR DE(W)HYDRAT?
L88	2911	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L87 AND L48
L89	279	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L88 AND L50
L90	17	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L89 AND L52
L91	1	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L89 AND L56
L92	16	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L89 AND L61
L93	1	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L89 AND L66
L94	2	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L89 AND L70
L95	31	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON (L90 OR L91 OR L92 OR L93 OR L94)
L97	279	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L88 AND L50
L98	17	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L97 AND L52
L100	1	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L98 AND L66
L101	1	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L98 AND L70
L102	1	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L97 AND L56
L103	1	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L97 AND L66
L104	2	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L97 AND L70
L105	19455	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L48 AND L52
L106	27	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L105 AND L56
L107	6	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L106 AND L66
L109	16	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L49 AND L56
L110	3	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L109 AND L66
L112	9	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L89 AND L54
L113	9	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L95 AND L54
L117	10	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON L112 OR (L100 OR L101 OR L102 OR L103 OR L104)

L118	15	SEA	FILE=HCAPLUS	ABB=ON PLU=ON	L117 OR L107 OR L110 OR L113
L119	57	SEA	FILE=HCAPLUS	ABB=ON PLU=ON	L118 OR L85
L121	35	SEA	FILE=HCAPLUS	ABB=ON PLU=ON	L49 AND L87
L122	5	SEA	FILE=HCAPLUS	ABB=ON PLU=ON	L121 AND L52
L123	1	SEA	FILE=HCAPLUS	ABB=ON PLU=ON	L121 AND L54
L124	1	SEA	FILE=HCAPLUS	ABB=ON PLU=ON	L121 AND L56
L125	1	SEA	FILE=HCAPLUS	ABB=ON PLU=ON	L121 AND L66
L126	2	SEA	FILE=HCAPLUS	ABB=ON PLU=ON	L121 AND L70
L127	5	SEA	FILE=HCAPLUS	ABB=ON PLU=ON	(L122 OR L123 OR L124 OR L125 OR L126)
L128	60	SEA	FILE=HCAPLUS	ABB=ON PLU=ON	L127 OR L119

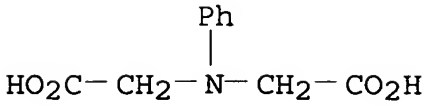
=> d l128 1-60 cbib abs hitstr hitind

L128 ANSWER 1 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
2005:660755 Document No. 143:142810 IR-laser-sensitive photopolymerizable compositions, and negative-working photoimaging materials for various uses including printing plates. Fujimaki, Kazuhiro (Fuji Photo Film Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 2005202314 A2 20050728, 84 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2004-10832 20040119.

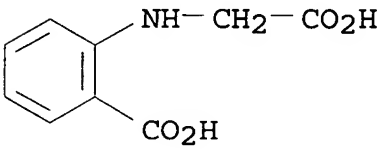
AB The compns. contain monocarboxylic acids, polycarboxylic acids, **IR-absorbing** agents, **radical polymerization initiators**, and ethylenic monomers, wherein the monocarboxylic acids and/or polycarboxylic acids bear groups expressed by XC(R1)(R2)CO2H [X = O, S, SO2, CO, NR3; R1-3 = H, monovalent nonmetallic substituent; R1 and R2, or R3 and R1 or R2 may form a ring]. Also claimed are the photoimaging materials containing the compns. on supports. The carboxylic acids work as stabilizer for the **polymerization** initiators without causing drop in sensitivity of the compns. themselves in long-period storage. Thus, a presensitized lithog. plate was manufactured by using the composition containing N-phenyliminodiacetic acid monoaniline amide.

IT **1137-73-1**, N-Phenyliminodiacetic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(in preparation of monocarboxylic acid; photopolymerizable composition containing mono- and polycarboxylic acids as **polymerization** catalyst stabilizers)

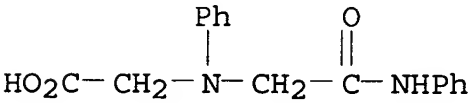
RN 1137-73-1 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-phenyl- (9CI) (CA INDEX NAME)



IT **612-42-0P 743422-98-2P**
RL: IMF (Industrial manufacture); MOA (Modifier or additive use); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(stabilizer for **polymerization** catalyst; photopolymerizable composition containing mono- and polycarboxylic acids as polymerization
catalyst stabilizers)
RN 612-42-0 HCAPLUS
CN Benzoic acid, 2-[(carboxymethyl)amino]- (9CI) (CA INDEX NAME)

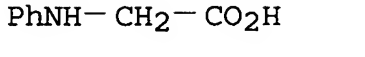


RN 743422-98-2 HCAPLUS
CN Glycine, N-[2-oxo-2-(phenylamino)ethyl]-N-phenyl- (9CI) (CA INDEX NAME)

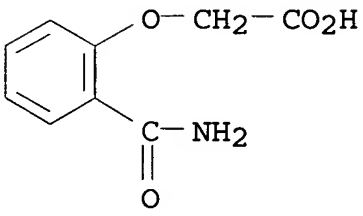


IT **103-01-5 25395-22-6 87964-30-5**
743423-02-1 858967-70-1 858967-73-4
858967-80-3 858967-83-6
RL: MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)
(stabilizer for **polymerization** catalyst; photopolymerizable composition containing mono- and polycarboxylic acids as polymerization
catalyst stabilizers)
RN 103-01-5 HCAPLUS

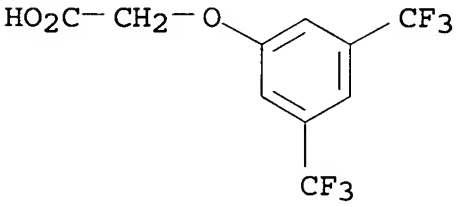
CN Glycine, N-phenyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



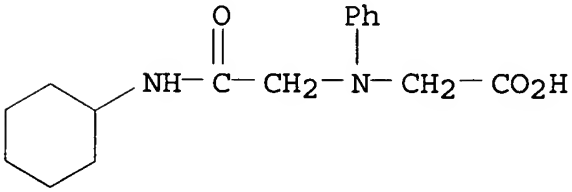
RN 25395-22-6 HCAPLUS
CN Acetic acid, [2-(aminocarbonyl)phenoxy]- (9CI) (CA INDEX NAME)



RN 87964-30-5 HCAPLUS
CN Acetic acid, [3,5-bis(trifluoromethyl)phenoxy]- (9CI) (CA INDEX NAME)

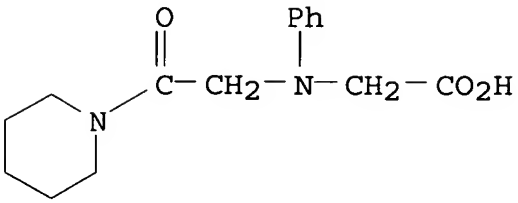


RN 743423-02-1 HCAPLUS
CN Glycine, N-[2-(cyclohexylamino)-2-oxoethyl]-N-phenyl- (9CI) (CA INDEX NAME)

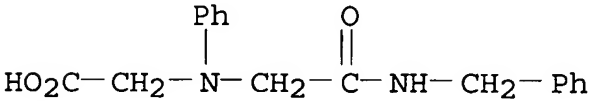


RN 858967-70-1 HCAPLUS

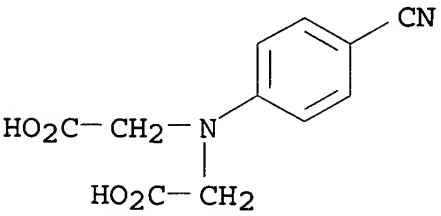
CN Glycine, N-[2-oxo-2-(1-piperidinyl)ethyl]-N-phenyl- (9CI) (CA INDEX NAME)



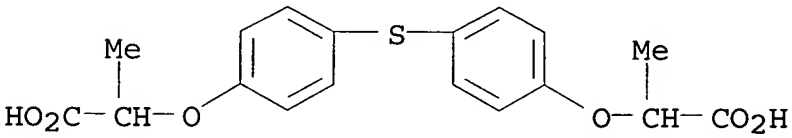
RN 858967-73-4 HCAPLUS
CN Glycine, N-[2-oxo-2-[(phenylmethyl)amino]ethyl]-N-phenyl- (9CI) (CA INDEX NAME)



RN 858967-80-3 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-(4-cyanophenyl)- (9CI) (CA INDEX NAME)



RN 858967-83-6 HCAPLUS
CN INDEX NAME NOT YET ASSIGNED



IC ICM G03F007-004

ICS C08F002-44; G03F007-00
CC 74-6 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 25, 38
IT Stabilizing agents
(for photopolymn. catalysts; photopolymerizable composition containing
mono- and polycarboxylic acids as **polymerization** catalyst stabilizers)
IT Photoimaging materials
(photopolymerizable; photopolymerizable composition containing mono- and
polycarboxylic acids as **polymerization** catalyst stabilizers)
IT Lithographic plates
(presensitized; photopolymerizable composition containing mono- and polycarboxylic acids as **polymerization** catalyst stabilizers)
IT 79-08-3, Bromoacetic acid 118-92-3, 2-Aminobenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(in preparation of dicarboxylic acid; photopolymerizable composition containing
mono- and polycarboxylic acids as **polymerization** catalyst stabilizers)
IT 62-53-3, Aniline, reactions **1137-73-1**,
N-Phenyliminodiacetic acid 56956-66-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(in preparation of monocarboxylic acid; photopolymerizable composition
containing mono- and polycarboxylic acids as **polymerization** catalyst stabilizers)
IT **612-42-0P 743422-98-2P**
RL: IMF (Industrial manufacture); MOA (Modifier or additive use); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(stabilizer for **polymerization** catalyst; photopolymerizable composition containing mono- and polycarboxylic acids as polymerization
catalyst stabilizers)
IT 88-99-3, 1,2-Benzenedicarboxylic acid, uses **103-01-5**
4282-31-9, 2,5-Thiophenedicarboxylic acid **25395-22-6**
87964-30-5 743423-02-1 858967-70-1
858967-73-4 858967-80-3 858967-83-6
RL: MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)
(stabilizer for **polymerization** catalyst; photopolymerizable composition containing mono- and polycarboxylic acids as polymerization

catalyst stabilizers)

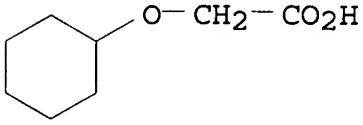
L128 ANSWER 2 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
2005:408526 Document No. 142:438732 Lithographic plates showing high sensitivity for direct IR-laser platemaking and good printability and yellow light-resistant photopolymerizable compositions therefor. Kakino, Ryuki; Kunita, Kazuto; Fujimaki, Kazuhiro (Fuji Photo Film Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 2005122038 A2 20050512, 86 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2003-359350 20031020.

AB The compns. contain (A) ZYXCR1R2CO2H (R1, R2 = H, monovalent substituent; X = O, S, SO2, NR3; R3 = H, monovalent substituent other than aromatic; Y = divalent linking group containing no aromatic ring in main chain; Z = aromatic) or WXCR1R2CO2H (R1, R2, X = same as above; W = H, same as R3), (B) **polymerizable** compds., (C) **radical initiators**, and optionally (D) **IR absorbers.** Also claimed are lithog. plates having recording layers of the above compns. on supports.

IT **71995-54-5**
RL: MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)
(yellow light-resistant photopolymerizable compns. for lithog. plates with high sensitivity for direct IR-laser platemaking and good printability)

RN 71995-54-5 HCAPLUS

CN Acetic acid, (cyclohexyloxy)- (6CI, 9CI) (CA INDEX NAME)



IC ICM G03F007-004
ICS C08F002-44; G03F007-00

CC 74-6 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 38

IT Optical materials
(**IR absorbers**; yellow light-resistant photopolymerizable compns. for lithog. plates with high sensitivity for direct IR-laser platemaking and good printability)

IT **IR** materials
(**absorbers**; yellow light-resistant photopolymerizable compns. for lithog. plates with high sensitivity for direct IR-laser platemaking and good printability)

IT 110992-66-0 110992-87-5
RL: MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)
(**IR absorbers**; yellow light-resistant photopolymerizable compns. for lithog. plates with high sensitivity for direct IR-laser platemaking and good printability)

IT 676349-80-7 790225-29-5
RL: CAT (Catalyst use); TEM (Technical or engineered material use); USES (Uses)
(**radical polymerization initiators**; yellow light-resistant photopolymerizable compns. for lithog. plates with high sensitivity for direct IR-laser platemaking and good printability)

IT 54884-96-7 **71995-54-5** 147974-54-7 220335-84-2
850754-51-7 850754-52-8 850754-53-9 850754-54-0 850754-55-1
850754-56-2 850754-57-3 850754-58-4
RL: MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)
(yellow light-resistant photopolymerizable compns. for lithog. plates with high sensitivity for direct IR-laser platemaking and good printability)

L128 ANSWER 3 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
2005:335705 Document No. 143:44104 Mechanistic Study of Photoinitiated Free Radical **Polymerization** Using Thioxanthone Thioacetic Acid as One-Component Type II Photoinitiator. Aydin, Meral; Arsu, Nergis; Yagci, Yusuf; Jockusch, Steffen; Turro, Nicholas J. (Department of Chemistry, Yildiz Technical University, Istanbul, 34210, Turk.). Macromolecules, 38(10), 4133-4138 (English) 2005. CODEN: MAMOBX. ISSN: 0024-9297. Publisher: American Chemical Society.

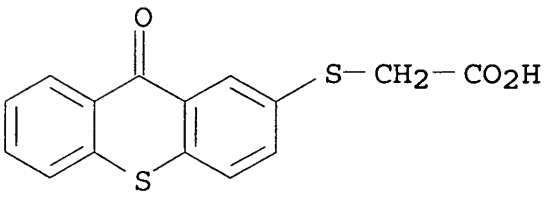
AB A mechanistic study concerning photoinitiated free radical **polymerization** using thioxanthone thioacetic acid (TX-S-CH2-COOH) as one-component Type II photoinitiator was performed. Steady-state and time-resolved fluorescence and phosphorescence spectroscopy, as well as laser flash photolysis was employed to study the photophysics and photochem. of TX-S-CH2-COOH. The initiator undergoes efficient intersystem crossing into the triplet state and the lowest triplet state possesses π-π^* configuration. In contrast to the unsubstituted thioxanthone, TX-S-CH2-COOH shows an

unusually short triplet lifetime (65 ns) indicating an intramol. reaction. From fluorescence, phosphorescence, and laser flash photolysis studies, in conjunction with photopolymn. expts., we propose that TX-S-CH2-COOH triplets undergo intramol. electron transfer followed by hydrogen abstraction and **decarboxylation** producing alkyl radicals, which are the active **initiator radicals** in photoinduced **polymerization** At low initiator concns. (below 5 + 10-3 M) this intramol. reaction is the dominant path. At concns. above 5 + 10-3 M, however, the resp. intermol. reactions may be operative.

IT **620170-13-0**
RL: CAT (Catalyst use); PRP (Properties); USES (Uses)
(mechanistic study of photoinitiated free radical **polymn** . of Me methacrylate using thioxanthone thioacetic acid as one-component Type II photoinitiator)

RN 620170-13-0 HCAPLUS

CN Acetic acid, [(9-oxo-9H-thioxanthen-2-yl)thio]- (9CI) (CA INDEX NAME)



CC 35-3 (Chemistry of Synthetic High Polymers)

ST thioxanthone thioacetic acid photoinitiator radical **polymn** photolysis fluorescence phosphorescence

IT Fluorescence
Luminescence
Optical absorption
(mechanistic study of photoinitiated free radical **polymn** . of Me methacrylate using thioxanthone thioacetic acid as one-component Type II photoinitiator)

IT **Polymerization**
Polymerization catalysts
(photochem., radical; mechanistic study of photoinitiated free radical **polymerization** of Me methacrylate using thioxanthone thioacetic acid as one-component Type II photoinitiator)

IT **620170-13-0**
RL: CAT (Catalyst use); PRP (Properties); USES (Uses)

(mechanistic study of photoinitiated free radical **polymn**. of Me methacrylate using thioxanthone thioacetic acid as one-component Type II photoinitiator)

IT 9011-14-7P, Poly(methyl methacrylate)
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(mechanistic study of photoinitiated free radical **polymn**. of Me methacrylate using thioxanthone thioacetic acid as one-component Type II photoinitiator)

L128 ANSWER 4 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
2005:212591 Document No. 142:306466 Photopolymerizable photoimaging composition and negatively-working directly-imaging lithographic printing plate precursors therefrom. Fujimaki, Kazuhiro (Fuji Photo Film Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 2005062482 A2 20050310, 81 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2003-292530 20030812.

AB The title composition contains a **radical polymerization initiator**, a **radical polymerization** co-**initiator** of ≤1.10 V oxidation potential, an **IR-absorber**, and radically **polymerizable** compds. The composition shows high sensitivity and good storageability and provides highly durable layers.

IT **19525-59-8D, radical polymerization** co-**initiator**
RL: CAT (Catalyst use); USES (Uses)
(**radical polymerization** co-**initiator** in composition)

RN 19525-59-8 HCAPLUS
CN Glycine, N-phenyl-, monopotassium salt (8CI, 9CI) (CA INDEX NAME)

PhNH—CH_2—CO_2H

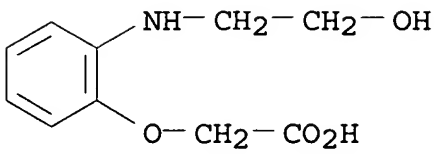
● K

IC ICM G03F007-029
ICS C08F002-44; C08F002-50; G03F007-004; G03F007-00
CC 74-6 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
IT 110992-87-5 603959-43-9 835902-38-0
RL: TEM (Technical or engineered material use); USES (Uses)

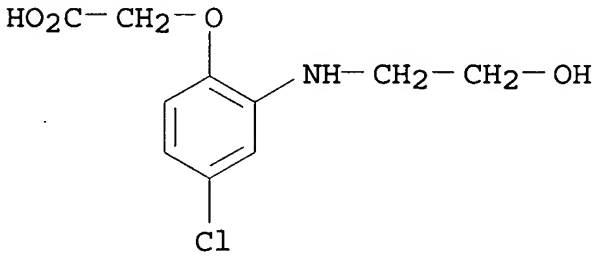
(**IR-absorber** in composition)
IT 603-34-9D, **radical polymerization** co-**initiator**
1628-58-6D, **radical polymerization** co-**initiator**
19525-59-8D, **radical polymerization** co-**initiator** 511304-75-9D, **radical polymn**. co-**initiator** 847573-63-1D, **radical polymerization** co-**initiator** 847573-64-2D, **radical polymerization** co-**initiator**
847590-95-8D, **radical polymerization** co-**initiator** 847590-96-9D, **radical polymn**. co-**initiator** 847590-98-1D, **radical polymerization** co-**initiator** 847590-99-2D, **radical polymerization** co-**initiator**
847591-01-9D, **radical polymerization** co-**initiator** 847591-02-0D, **radical polymn**. co-**initiator**
RL: CAT (Catalyst use); USES (Uses)
(**radical polymerization** co-**initiator** in composition)
IT 676349-78-3 761432-18-2 790225-29-5
RL: CAT (Catalyst use); USES (Uses)
(**radical polymerization initiator** in composition)
IT 29570-58-9 80937-22-0 91105-84-9 761432-20-6 847565-07-5
847573-65-3
RL: TEM (Technical or engineered material use); USES (Uses)
(radically **polymerizable** compds. in composition)

L128 ANSWER 5 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
2005:209978 Document No. 142:306465 Photopolymerizable photoimaging composition and negatively-working directly-imaging lithographic printing plate precursors made thereof. Fujimaki, Kazuhiro (Fuji Photo Film Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 2005062478 A2 20050310, 81 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2003-292453 20030812.
AB The title composition contains a compound with an amino groups and hydroxy
groups, an **IR-absorber**, a **radical polymerization initiator**, and ethylenic unsatd. compds. The composition shows high sensitivity and good storageability and provides highly durable layers.
IT **847564-92-5 847564-95-8**
RL: TEM (Technical or engineered material use); USES (Uses)
(compound with an amino groups and hydroxy groups in composition)
RN 847564-92-5 HCAPLUS

CN Acetic acid, [2-[(2-hydroxyethyl)amino]phenoxy]- (9CI) (CA INDEX NAME)



RN 847564-95-8 HCAPLUS
CN Acetic acid, [4-chloro-2-[(2-hydroxyethyl)amino]phenoxy]- (9CI) (CA INDEX NAME)

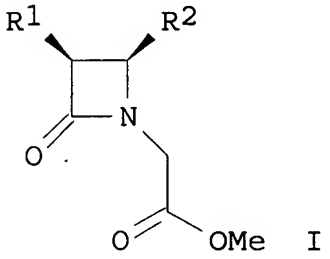


IC ICM G03F007-004
ICS C08F002-44; G03F007-00
CC 74-6 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
IT 110992-87-5 835902-38-0
RL: TEM (Technical or engineered material use); USES (Uses)
(**IR-absorber** in composition)
IT 93-90-3 102-71-6, uses 111-42-2, uses 120-07-0 122-96-3, 1,4-Piperazinediethanol 140-07-8 732-51-4 3040-44-6, 1-Piperidineethanol 6303-96-4 6315-51-1 13127-77-0 19721-54-1 27076-96-6 71345-85-2 89943-04-4 91645-48-6 121459-15-2, 1H-Indole-1-ethanol 847564-87-8 **847564-92-5** 847564-93-6 **847564-95-8**
RL: TEM (Technical or engineered material use); USES (Uses)
(compound with an amino groups and hydroxy groups in composition)
IT 120307-06-4 253585-83-0 603959-43-9 676349-78-3 761432-18-2 790225-29-5 847565-03-1
RL: TEM (Technical or engineered material use); USES (Uses)
(**radical polymerization initiator** in

composition)

L128 ANSWER 6 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
2005:127618 Document No. 142:355068 Exploring the Solid-Phase Synthesis of 3,4-Disubstituted β-Lactams: Scope and Limitations. Delpiccolo, Carina M. L.; Mendez, Luciana; Fraga, M. Amelia; Mata, Ernesto G. (Instituto de Quimica Organica de Sintesis (CONICET - UNR), Facultad de Ciencias Bioquimicas y Farmaceuticas, Universidad Nacional de Rosario, Rosario, 2000, Argent.). Journal of Combinatorial Chemistry, 7(2), 331-344 (English) 2005. CODEN: JCCHFF. ISSN: 1520-4766. Publisher: American Chemical Society.

GI



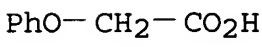
I

AB This work describes a comprehensive study on the solid-phase synthesis of 3,4-disubstituted β-lactams, e.g. I [R1 = PhO, phthaloyl, MeO, R2 = 3,4-(MeO)2C6H3, Ph, 4-MeOC6H4, (E)-PhCH:CH, 2-furyl, 4-BrC6H4, 4-MeC6H4, 4-ClC6H4, 2-BrC6H4]. In situ generated ketenes react with immobilized aldimines, e.g. R2CH:NCH2CO2W (W = Wang resin), under mild conditions to generate libraries of β-lactams in good to very good overall isolated yields. Different com. available solid supports were studied, with the cost-effective Wang resin proving to be the most effective. The utility of the protocol was also demonstrated by the highly efficient asym. versions when homochiral ketenes or homochiral aldimines were used. A practical technique for the preparation of manual solid-phase parallel libraries of biol. interesting β-lactam compds., using Mukaiyama's salt as **dehydrating** agent, is also presented. Reactions were easily monitored by FT-IR and **gel**-phase 13C NMR using conventional equipment.

IT **122-59-8**, Phenoxyacetic acid
RL: CRT (Combinatorial reactant); RCT (Reactant); CMBI (Combinatorial study); RACT (Reactant or reagent)

(solid-phase synthesis of 3,4-disubstituted β-lactams, use of Staudinger reaction, and asym. version)

RN 122-59-8 HCAPLUS
CN Acetic acid, phenoxy- (8CI, 9CI) (CA INDEX NAME)



CC 26-5 (Biomolecules and Their Synthetic Analogs)
IT 98-01-1, 2-Furancarboxaldehyde, reactions 100-52-7, Benzaldehyde, reactions 104-87-0, 4-Methylbenzaldehyde 104-88-1, 4-Chlorobenzaldehyde, reactions 120-14-9, 3,4-Dimethoxybenzaldehyde **122-59-8**, Phenoxyacetic acid 123-11-5, 4-Methoxybenzaldehyde, reactions 701-99-5, Phenoxyacetyl chloride 1122-91-4, 4-Bromobenzaldehyde 3724-65-0, Crotonic acid 4530-20-5D, Merrifield resin-supported 4530-20-5D, PAM resin-supported 4702-13-0, Phthalimidoacetic acid 6630-33-7, 2-Bromobenzaldehyde 6780-38-7, Phthalimidoacetyl chloride 14371-10-9, (E)-3-Phenyl-2-propenal 29022-11-5D, Wang-resin supported 38870-89-2, Methoxyacetyl chloride 76640-41-0D, Merrifield resin-supported 76640-41-0D, PAM resin-supported 82934-67-6D, Merrifield resin-supported 82934-67-6D, PAM resin-supported 99333-54-7 375365-51-8D, Wang-resin supported 515158-60-8D, Wang-resin supported 529485-93-6D, Wang resin-supported 849231-97-6D, Wang resin-supported
RL: CRT (Combinatorial reactant); RCT (Reactant); CMBI (Combinatorial study); RACT (Reactant or reagent)
(solid-phase synthesis of 3,4-disubstituted β-lactams, use of Staudinger reaction, and asym. version)

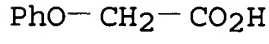
L128 ANSWER 7 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
2004:799820 Document No. 142:482359 Novel dissociative electron transfer photoinitiators for free radical **polymerization.** Wrzyszczynski, Andrzej; Paczkowski, Jerzy (Fac. of Chem. Technol. and Eng., Univ. of Technol. and Agriculture, Bydgoszcz, 85-326, Pol.). Polimery (Warsaw, Poland), 49(9), 606-614 (English) 2004. CODEN: POLIA4. ISSN: 0032-2725. Publisher: Instytut Chemii Przemyslowej.
AB Radical **polymerization** of 2-ethyl-2-(hydroxymethyl)-1,3-propanediol triacrylate (TMPTA), photoinduced with redox system: electron donor-absorber, was presented. Xanthene dyes: Rose bengal ditetrabutyl-ammonium salt [RBTBAS] and 5,7-diiodo-3-pentoxy-6-fluorone [DIPF] were used as absorbers. Electron donors in the system studied were: (phenylthio)acetic acid (PTAA),

(phenylthio)acetic acid tetrabutylammonium salt (PTAA AS), Et (phenylthio)acetate (PTAA EE) or n-butyltriphenyl borate (BuPh3B+). Photopolymn. mechanism was studied using laser flash photolysis method. Photoredn. with PTAA or PTAA AS goes with electron transfer from sulfur atom to dye in triplet state. In case when RBTBAS is used as electron acceptor the anionic radicals of the dye [RB•3- and RB•2-] are obtained. The presence of these anionic radicals shows that after electron transfer the carboxylic group exists in an ionic form what let intramol. electron transfer from carboxylate group to sulfur cationic radical, followed with rapid **decarboxylation.** As a result of **decarboxylation** the neutral thiomethylene radicals (Ph-S-CH2•) are formed which, after escape from solvent cage, take part in photoinitiation of the **polymerization** Transformation of sulfur(DIPF) containing carboxylic acids into their tetrabutylammonium salts significantly increases the sensitivity of the photoinitiating system. It also increases photopolymn. rate (Rp), which is a function of square root of the quantum yield of **decarboxylation** process (ϕCO2).

IT **122-59-8**, Phenoxyacetic acid
RL: CAT (Catalyst use); USES (Uses)
(electron donor; dissociative electron transfer photoinitiators for free radical **polymerization**)

RN 122-59-8 HCAPLUS

CN Acetic acid, phenoxy- (8CI, 9CI) (CA INDEX NAME)



CC 35-3 (Chemistry of Synthetic High Polymers)

ST dissociative electron transfer photoinitiator free radical **polymn**

IT **Polymerization**
Polymerization catalysts
Polymerization kinetics
(photochem., radical; dissociative electron transfer photoinitiators for free radical **polymerization**)

IT 97816-39-2 404384-36-7
RL: CAT (Catalyst use); USES (Uses)
(absorber; dissociative electron transfer photoinitiators for free radical **polymerization**)

IT 103-04-8, (Phenylthio)acetic acid **122-59-8**, Phenoxyacetic acid 7605-25-6, Ethyl (phenylthio)acetate 13205-48-6 16188-55-9, 4-(Methylthio)phenylacetic acid 610769-56-7 653593-61-4 653593-62-5 653593-63-6

RL: CAT (Catalyst use); USES (Uses)
(electron donor; dissociative electron transfer photoinitiators for free radical **polymerization**)

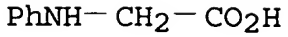
IT 15625-89-5, 2-Ethyl-2-(hydroxymethyl)-1,3-propanediol triacrylate
RL: RCT (Reactant); RACT (Reactant or reagent)
(monomer; dissociative electron transfer photoinitiators for free radical **polymerization**)

L128 ANSWER 8 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
2004:700261 Document No. 141:215685 **Polymerizable** composition and lithographic printing plate precursor. Fujimaki, Kazuhiro (Fuji Photo Film Co., Ltd., Japan). Eur. Pat. Appl. EP 1449651 A2 20040825, 96 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK. (English). CODEN: EPXXDW. APPLICATION: EP 2004-3844 20040220. PRIORITY: JP 2003-43087 20030220; JP 2003-194852 20030710.

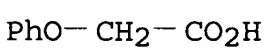
AB A **polymerizable** composition comprises: (A) a compound which causes at least one of **decarboxylation** and **dehydration** by heat; (B) a **radical initiator**; (C) a compound having at least one ethylenically unsatd. bond; and (D) an **IR** ray **absorber** and a lithog. printing plate precursor comprising a support and a recording layer comprising said **polymerizable** composition

IT **103-01-5 122-59-8 1137-73-1**
3959-23-7 35676-11-0 60085-74-7
161555-27-7 743422-66-4 743422-67-5
743422-68-6 743422-69-7 743422-70-0
743422-73-3 743422-75-5 743422-76-6
743422-77-7 743422-78-8 743422-79-9
743422-80-2 743422-81-3 743422-82-4
743422-83-5 743422-84-6 743422-85-7
743422-86-8 743422-88-0 743422-89-1
743422-90-4 743422-92-6 743422-93-7
743422-96-0 743422-98-2 743422-99-3
743423-00-9 743423-01-0 743423-02-1
743423-03-2
RL: TEM (Technical or engineered material use); USES (Uses)
(**polymerizable** composition and lithog. printing plate precursor containing)

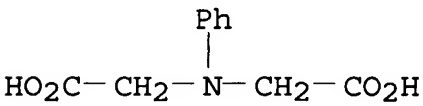
RN 103-01-5 HCAPLUS
CN Glycine, N-phenyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



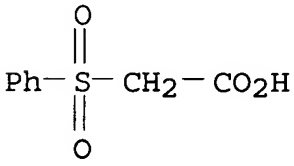
RN 122-59-8 HCAPLUS
CN Acetic acid, phenoxy- (8CI, 9CI) (CA INDEX NAME)



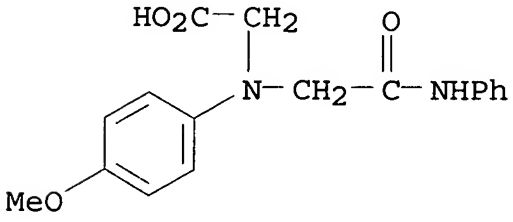
RN 1137-73-1 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-phenyl- (9CI) (CA INDEX NAME)



RN 3959-23-7 HCAPLUS
CN Acetic acid, (phenylsulfonyl)- (6CI, 8CI, 9CI) (CA INDEX NAME)

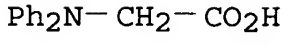


RN 35676-11-0 HCAPLUS
CN Glycine, N-(4-methoxyphenyl)-N-[2-oxo-2-(phenylamino)ethyl]- (9CI) (CA INDEX NAME)

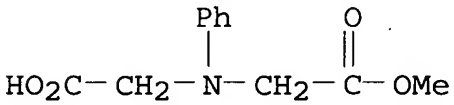


RN 60085-74-7 HCAPLUS

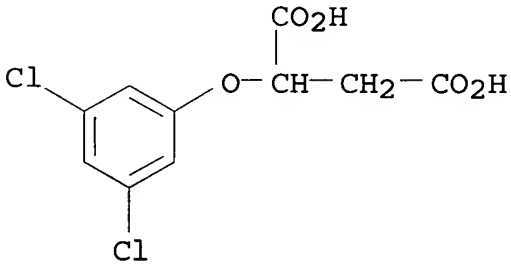
CN Glycine, N,N-diphenyl- (9CI) (CA INDEX NAME)



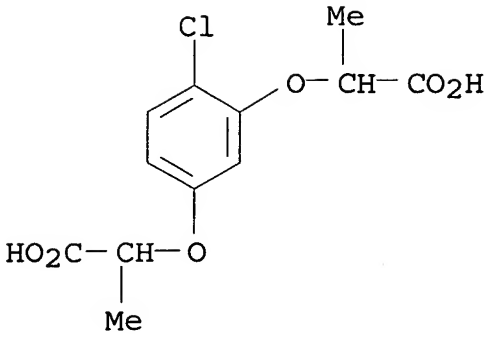
RN 161555-27-7 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-phenyl-, 1-methyl ester (9CI) (CA INDEX NAME)



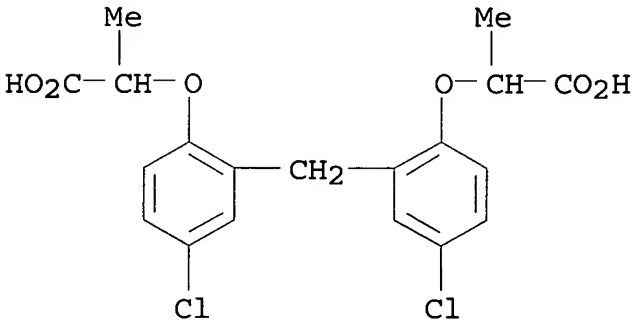
RN 743422-66-4 HCAPLUS
CN Butanedioic acid, (3,5-dichlorophenoxy)- (9CI) (CA INDEX NAME)



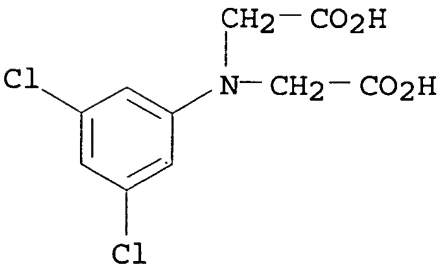
RN 743422-67-5 HCAPLUS
CN Propanoic acid, 2,2'-[(4-chloro-1,3-phenylene)bis(oxy)]bis- (9CI) (CA INDEX NAME)



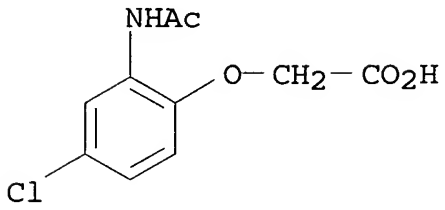
RN 743422-68-6 HCAPLUS
CN Propanoic acid, 2,2'-[methylenebis[(4-chloro-2,1-phenylene)oxy]]bis- (9CI) (CA INDEX NAME)



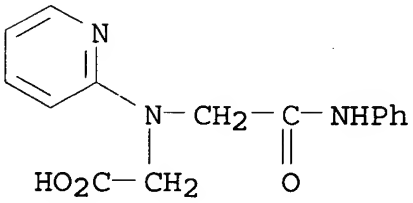
RN 743422-69-7 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-(3,5-dichlorophenyl)- (9CI) (CA INDEX NAME)



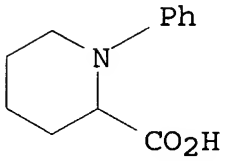
RN 743422-70-0 HCAPLUS
CN Acetic acid, [2-(acetylamino)-4-chlorophenoxy]- (9CI) (CA INDEX NAME)



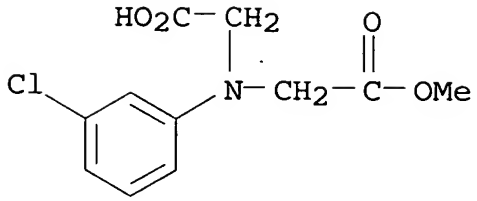
RN 743422-73-3 HCAPLUS
CN Glycine, N-[2-oxo-2-(phenylamino)ethyl]-N-2-pyridinyl- (9CI) (CA INDEX NAME)



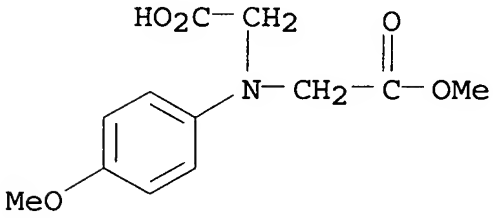
RN 743422-75-5 HCAPLUS
CN 2-Piperidinecarboxylic acid, 1-phenyl- (9CI) (CA INDEX NAME)



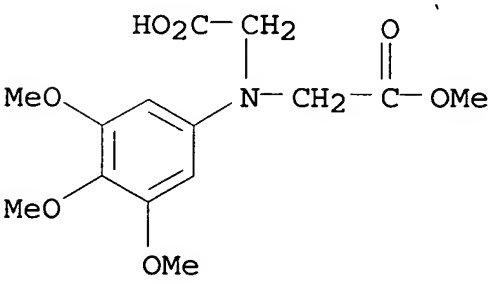
RN 743422-76-6 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-(3-chlorophenyl)-, 1-methyl ester (9CI) (CA INDEX NAME)



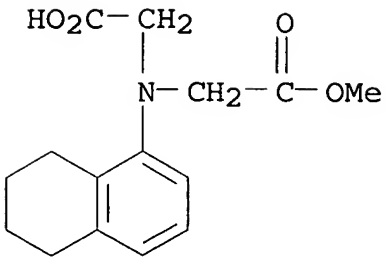
RN 743422-77-7 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-(4-methoxyphenyl)-, 1-methyl ester (9CI) (CA INDEX NAME)



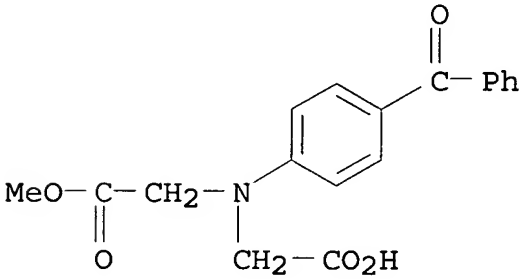
RN 743422-78-8 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-(3,4,5-trimethoxyphenyl)-, 1-methyl ester (9CI) (CA INDEX NAME)



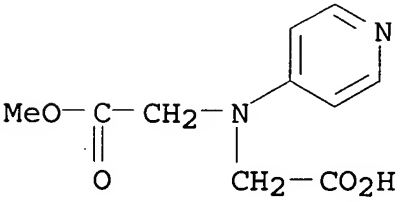
RN 743422-79-9 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-(5,6,7,8-tetrahydro-1-naphthalenyl)-, 1-methyl ester (9CI) (CA INDEX NAME)



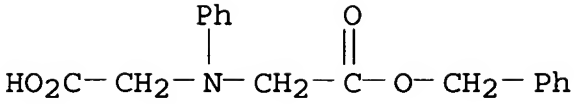
RN 743422-80-2 HCAPLUS
CN Glycine, N-(4-benzoylphenyl)-N-(carboxymethyl)-, 1-methyl ester (9CI) (CA INDEX NAME)



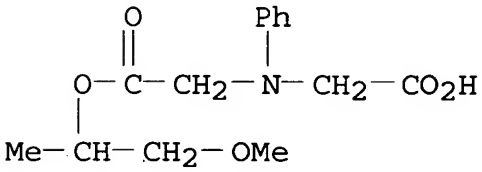
RN 743422-81-3 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-4-pyridinyl-, 1-methyl ester (9CI) (CA INDEX NAME)



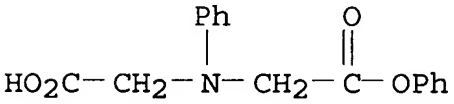
RN 743422-82-4 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-phenyl-, 1-(phenylmethyl) ester (9CI) (CA INDEX NAME)



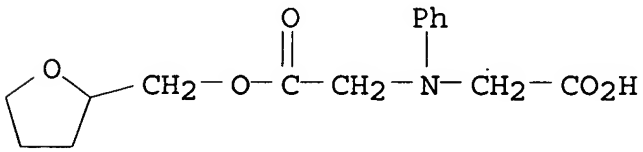
RN 743422-83-5 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-phenyl-, 1-(2-methoxy-1-methylethyl) ester (9CI) (CA INDEX NAME)



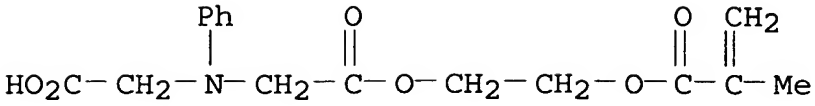
RN 743422-84-6 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-phenyl-, 1-phenyl ester (9CI) (CA INDEX NAME)



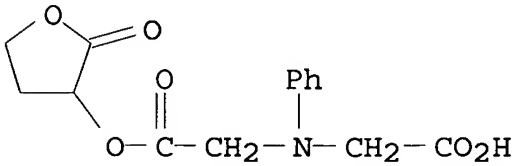
RN 743422-85-7 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-phenyl-, 1-[(tetrahydro-2-furanyl)methyl] ester (9CI) (CA INDEX NAME)



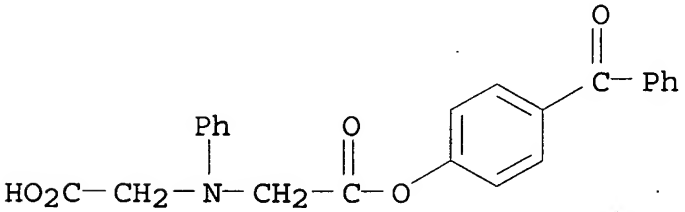
RN 743422-86-8 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-phenyl-, 1-[2-[(2-methyl-1-oxo-2-propenyl)oxy]ethyl] ester (9CI) (CA INDEX NAME)



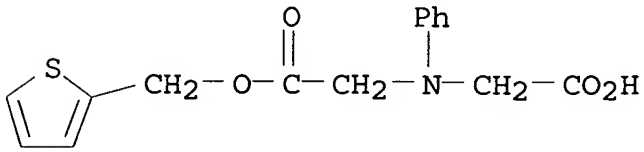
RN 743422-88-0 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-phenyl-, 1-(tetrahydro-2-oxo-3-furanyl) ester (9CI) (CA INDEX NAME)



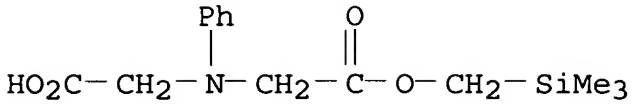
RN 743422-89-1 HCAPLUS
CN Glycine, N-[2-(4-benzoylphenoxy)-2-oxoethyl]-N-phenyl- (9CI) (CA INDEX NAME)



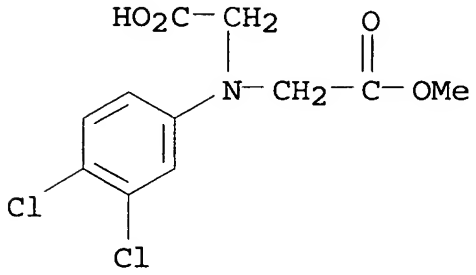
RN 743422-90-4 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-phenyl-, 1-(2-thienylmethyl) ester (9CI) (CA INDEX NAME)



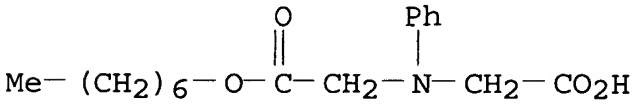
RN 743422-92-6 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-phenyl-, 1-[(trimethylsilyl)methyl] ester (9CI) (CA INDEX NAME)



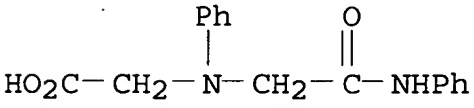
RN 743422-93-7 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-(3,4-dichlorophenyl)-, 1-methyl ester (9CI) (CA INDEX NAME)



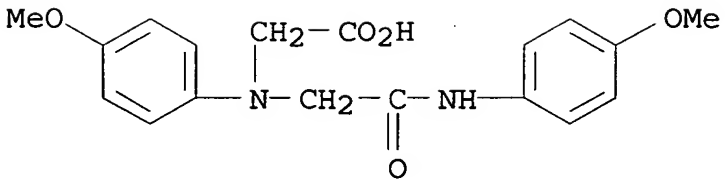
RN 743422-96-0 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-phenyl-, 1-heptyl ester (9CI) (CA INDEX NAME)



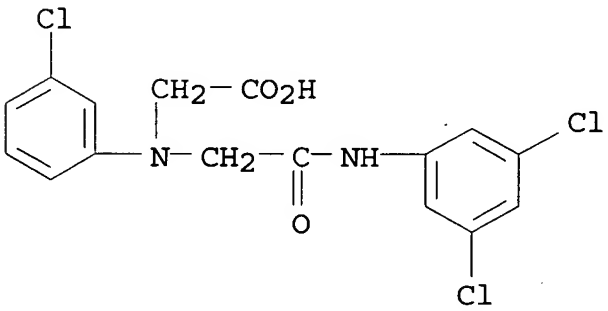
RN 743422-98-2 HCAPLUS
CN Glycine, N-[2-oxo-2-(phenylamino)ethyl]-N-phenyl- (9CI) (CA INDEX NAME)



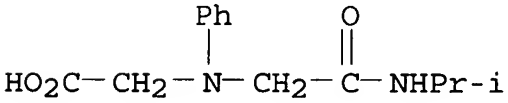
RN 743422-99-3 HCAPLUS
CN Glycine, N-(4-methoxyphenyl)-N-[2-[(4-methoxyphenyl)amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)



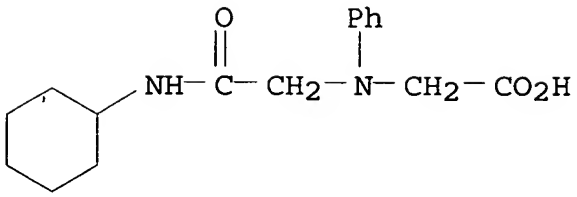
RN 743423-00-9 HCAPLUS
CN Glycine, N-(3-chlorophenyl)-N-[2-[(3,5-dichlorophenyl)amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)



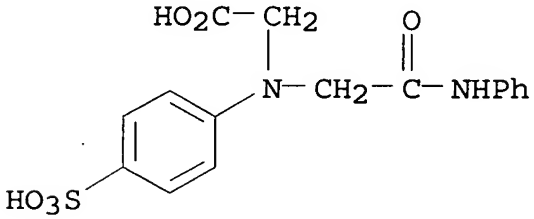
RN 743423-01-0 HCAPLUS
CN Glycine, N-[2-[(1-methylethyl)amino]-2-oxoethyl]-N-phenyl- (9CI) (CA INDEX NAME)



RN 743423-02-1 HCAPLUS
CN Glycine, N-[2-(cyclohexylamino)-2-oxoethyl]-N-phenyl- (9CI) (CA INDEX NAME)



RN 743423-03-2 HCAPLUS
CN Glycine, N-[2-oxo-2-(phenylamino)ethyl]-N-(4-sulfophenyl)- (9CI) (CA INDEX NAME)



IC ICM B41C001-10
ICS G03F007-004
CC **74-6** (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
ST **polymerizable** compn lithog printing plate precursor
IT Dyes
(**IR-absorbing; polymerizable** composition and lithog. printing plate precursor)
IT Lithographic plates
(**polymerizable** composition and lithog. printing plate precursor)
IT **103-01-5 122-59-8 1137-73-1**
3959-23-7 6915-15-7 **35676-11-0**
60085-74-7 62952-26-5 **161555-27-7**
743422-66-4 743422-67-5 743422-68-6
743422-69-7 743422-70-0 743422-71-1
743422-72-2 **743422-73-3** 743422-74-4 **743422-75-5**
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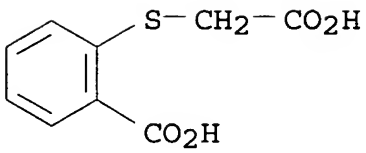
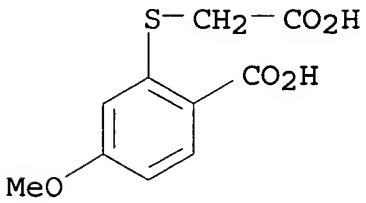
743422-99-3 743423-00-9 743423-01-0
743423-02-1 743423-03-2
RL: TEM (Technical or engineered material use); USES (Uses)
(**polymerizable** composition and lithog. printing plate precursor containing)

L128 ANSWER 9 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
2004:422850 Document No. 141:140865 Polythienobenzothiophenes, a new family of electroactive polymers: electrosynthesis, spectral characterization and modelling. Fouad, Irari; Mechbal, Zouhair; Chane-Ching, Kathleen I.; Adenier, Alain; Maurel, Francois; Aaron, Jean-Jacques; Vodicka, Petr; Cernovska, Katerina; Kozmik, Vaclav; Svoboda, Jiri (ITODYS, Universite Paris 7-Denis Diderot, Paris, 75005, Fr.). Journal of Materials Chemistry, 14(11), 1711-1721 (English) 2004. CODEN: JMACEP. ISSN: 0959-9428. Publisher: Royal Society of Chemistry.
AB Conducting polymers, including poly[thieno[3,2-b][1]benzothiophene] (poly-TBT) and poly[6-methoxythieno[3,2-b][1]benzothiophene] (poly-MeOTBT) were prepared electrochem. **polymerization** under anodic oxidation of the corresponding monomers in 0.1 M LiClO4/acetonitrile electrolyte solution The poly-TBT and poly-MeOTBT electroactive films were formed on platinum electrodes and characterized spectroscopically. FT-**IR** studies show that both polymers present coupling of the thiophene moiety and the Ph ring, with a step-like structure. MALDI-TOF mass spectrometry indicates that poly-TBT and poly-MeOTBT films are mainly constituted of short-chain oligomers. The results of MO calcns. performed on the basis of a radical-cation electropolymn. mechanism are in good agreement with spectral data.
IT **135-13-7**, 2-[(Carboxymethyl)thio]benzoic acid
103203-39-0, 2-[(Carboxymethyl)thio]-4-methoxybenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of monomers and mechanism of electrooxidative **polymerization** of thienobenzothiophenes and chain structure study using MO calcns. and MALDI-TOF)
RN 135-13-7 HCAPLUS
CN Benzoic acid, 2-[(carboxymethyl)thio]- (9CI) (CA INDEX NAME)



RN 103203-39-0 HCAPLUS
CN Benzoic acid, 2-[(carboxymethyl)thio]-4-methoxy- (9CI) (CA INDEX NAME)



CC 35-7 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 36, 76
ST thienobenzothiophene electrochem **polymn** anodic oxidn chain structure; methoxythienobenzothiophene polythiophene prepn structure MALDI TOF
IT Hydrolysis
(base; preparation of monomers and mechanism of electrooxidative **polymerization** of thienobenzothiophenes and chain structure study using MO calcns. and MALDI-TOF)
IT Polymers, preparation
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(conjugated, thieno-benzothiophenes; preparation of monomers and mechanism of electrooxidative **polymerization** of thienobenzothiophenes and chain structure study using MO calcns. and MALDI-TOF)
IT **Polymerization**
(electrochem., oxidative; preparation of monomers and mechanism of electrooxidative **polymerization** of thienobenzothiophenes and chain structure study using MO calcns. and MALDI-TOF)
IT Redox reaction
(electrochem., reversible; preparation of monomers and mechanism of electrooxidative **polymerization** of thienobenzothiophenes and chain structure study using MO calcns. and MALDI-TOF)

IT SOMO (molecular orbital)
(of radical cations in chain; preparation of monomers and mechanism of electrooxidative **polymerization** of thienobenzothiophenes and chain structure study using MO calcns. and MALDI-TOF)
IT Conducting polymers
(polythiophenes, thienobenzothiophenes; preparation of monomers and mechanism of electrooxidative **polymerization** of thienobenzothiophenes and chain structure study using MO calcns. and MALDI-TOF)
IT Alkylation
Chlorination
Cyclization
Decarboxylation
Electronic transition
Formylation
IR spectra
Optical absorption
(preparation of monomers and mechanism of electrooxidative **polymerization** of thienobenzothiophenes and chain structure study using MO calcns. and MALDI-TOF)
IT Polymer chains
(short-segment structure; preparation of monomers and mechanism of electrooxidative **polymerization** of thienobenzothiophenes and chain structure study using MO calcns. and MALDI-TOF)
IT Molecular orbital
(valence, radical-cation; preparation of monomers and mechanism of electrooxidative **polymerization** of thienobenzothiophenes and chain structure study using MO calcns. and MALDI-TOF)
IT 12597-70-5, Copper bronze
RL: CAT (Catalyst use); USES (Uses)
(**decarboxylation** catalyst; preparation of monomers and mechanism of electrooxidative **polymerization** of thienobenzothiophenes and chain structure study using MO calcns. and MALDI-TOF)
IT 30126-05-7P, Thieno[3,2-b][1]benzothiophene-2-carboxylic acid 694458-11-2P, Methyl thieno[3,2-b][1]benzothiophene-2-carboxylate 725737-29-1P, Methyl 6-methoxythieno[3,2-b][1]benzothiophene-2-carboxylate 725737-30-4P, 6-Methoxythieno[3,2-b][1]benzothiophene-2-carboxylic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of monomers and mechanism of electrooxidative **polymerization** of thienobenzothiophenes and chain structure study using MO calcns. and MALDI-TOF)

IT 247-52-9P, Thieno[3,2-b][1]benzothiophene 725737-31-5P, 6-Methoxythieno[3,2-b][1]benzothiophene
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(monomer; preparation of monomers and mechanism of electrooxidative **polymerization** of thienobenzothiophenes and chain structure study using MO calcns. and MALDI-TOF)

IT 75-05-8, Acetonitrile, uses 7791-03-9, Lithium perchlorate (LiClO4)
RL: NUU (Other use, unclassified); USES (Uses)
(**polymerization** and redox cycling electrolyte containing; preparation of monomers and mechanism of electrooxidative **polymerization** of thienobenzothiophenes and chain structure study using MO calcns. and MALDI-TOF)

IT 501332-77-0P, Thieno[3,2-b][1]benzothiophene homopolymer 725737-32-6P, 6-Methoxythieno[3,2-b][1]benzothiophene homopolymer
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of monomers and mechanism of electrooxidative **polymerization** of thienobenzothiophenes and chain structure study using MO calcns. and MALDI-TOF)

IT **135-13-7**, 2-[(Carboxymethyl)thio]benzoic acid 2365-48-2, Methyl thioglycolate 10025-87-3, Phosphoric trichloride **103203-39-0**, 2-[(Carboxymethyl)thio]-4-methoxybenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of monomers and mechanism of electrooxidative **polymerization** of thienobenzothiophenes and chain structure study using MO calcns. and MALDI-TOF)

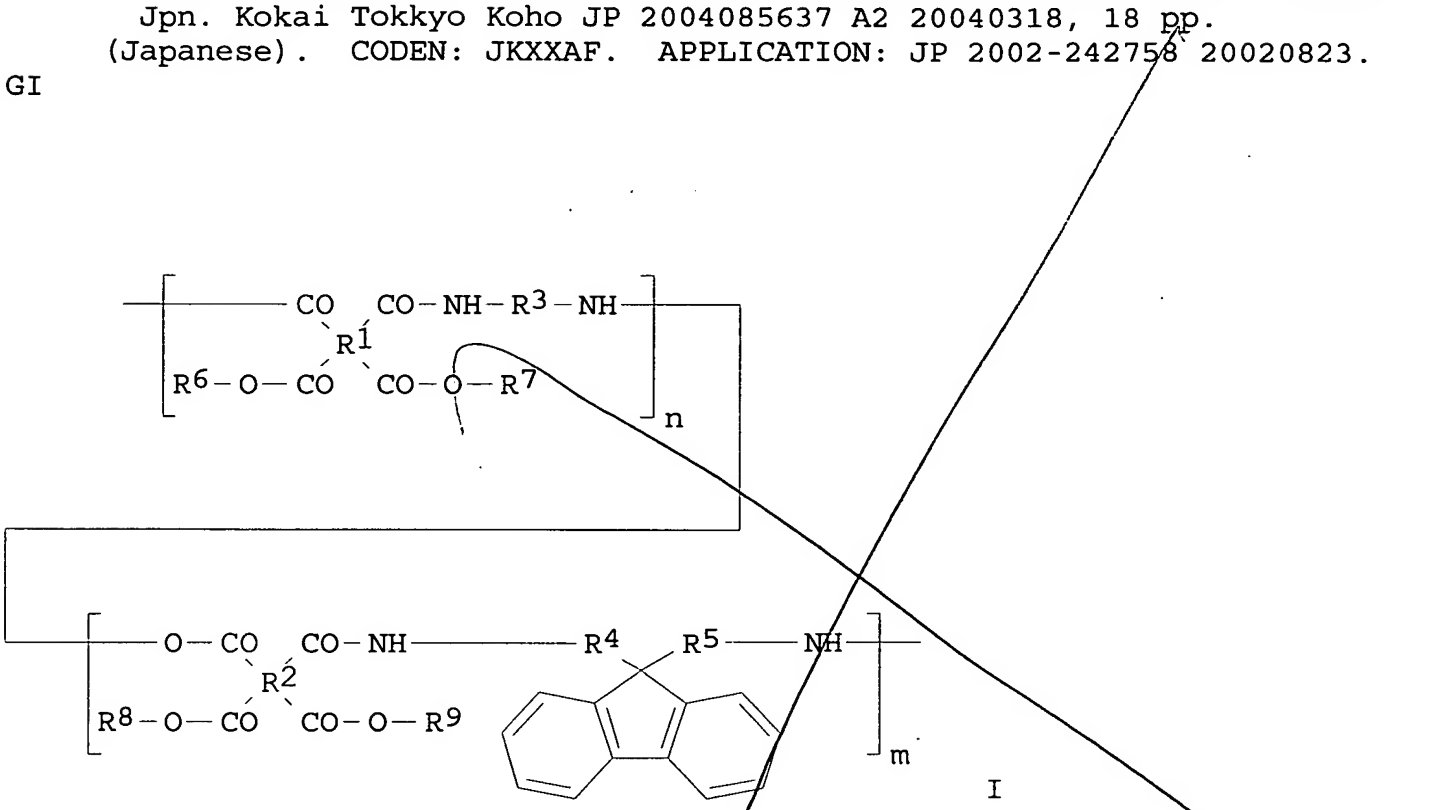
IT 14006-54-3P, 3-Chloro-2-benzothiophenecarboxaldehyde 725737-28-0P, 3-Chloro-6-methoxy[1]benzothiophene-2-carboxaldehyde
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of monomers and mechanism of electrooxidative **polymerization** of thienobenzothiophenes and chain structure study using MO calcns. and MALDI-TOF)

IT 1310-73-2, Sodium hydroxide, reactions
RL: RGT (Reagent); RACT (Reactant or reagent)
(preparation of monomers and mechanism of electrooxidative **polymerization** of thienobenzothiophenes and chain structure study using MO calcns. and MALDI-TOF)

L128 ANSWER 10 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
2004:219174 Document No. 140:278414 Negatively-working photosensitive fluorenyl-containing polyimide precursor composition and manufacture

of the composition. Hojo, Yasuhiro (Kyocera Chemical Corp., Japan). Jpn. Kokai Tokkyo Koho JP 2004085637 A2 20040318, 18 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2002-242758 20020823.

GI



I

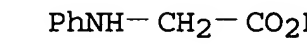
AB The composition contains a polyimide precursor I [R1, R2 = tetravalent aromatic group, tetravalent group made of aromatic rings linked through single bond, O, CO, SO2, CH2, C(CF3)2; R3-R5 = divalent aromatic group, divalent organic group made of aromatic rings linked through single bond, O, CO, SO2, CH2, C(CF3)2; R6-R9 = monovalent organic group involving ≥1 ethylenic unsatd. bond; m, n ≥1], a **dehydration** condensation agent for ring closure of the precursor, an agent for enhancing sensitivity to radiation, and a solvent. The composition is manufactured by the process involving (a) esterifying of an acid dianhydride with an unsatd. ester both corresponding to I, (b) polycondensing of the resulting ester and a diamine containing fluorenyl group corresponding to I in the presence of the **dehydrating** agent, (c) refining of the precursor, and (d) adding of the sensitizer. The composition is capable of patterning

by exposure to far UV at 365 nm.

IT **103-01-5**, N-Phenylglycine
RL: CAT (Catalyst use); USES (Uses)
(sensitizer; in neg.-working photosensitive fluorenyl-containing polyimide precursor composition)

RN 103-01-5 HCAPLUS

CN Glycine, N-phenyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IC ICM G03F007-027
ICS C08G073-10; G03F007-004; G03F007-038; H01L021-027; H01L021-312

CC **74-4** (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 38, 76

IT **Dehydration** reaction
(agents; in neg.-working photosensitive fluorenyl-containing polyimide precursor composition)

IT 111160-56-6
RL: RGT (Reagent); RACT (Reactant or reagent)
(**dehydrating** agent; in neg.-working photosensitive fluorenyl-containing polyimide precursor composition)

IT 66251-40-9P, Hexanediol diacrylate-2-hydroxyethyl methacrylate copolymer 87245-04-3P
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(in neg.-working **cured** fluorenyl-containing polyimide composition)

IT **103-01-5**, N-Phenylglycine
RL: CAT (Catalyst use); USES (Uses)
(sensitizer; in neg.-working photosensitive fluorenyl-containing polyimide precursor composition)

L128 ANSWER 11 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

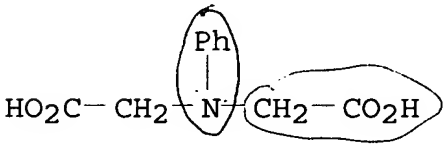
2003:967946 Document No. 140:21303 Planographic printing plate precursor. Goto, Takahiro (Fuji Photo Film Co., Ltd., Japan). Eur. Pat. Appl. EP 1369232 A1 20031210, 29 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK. (English). CODEN: EPXXDW. APPLICATION: EP 2003-12196 20030605. PRIORITY: JP 2002-164700 20020605.

AB The neg. planog. printing plate precursor for IR exposure has an image recording layer containing an **IR absorbing**

agent, a radical generator and a radical **polymerizable** compound on a support; the sensitivity ratio (S1/S60) is ≥0.5 and <1.0 in the image recording layer where S60 is the sensitivity when developed 60 min after IR laser exposure and S1 is the sensitivity when developed one minute after exposure. It is preferable that this composition also contains a polymer compound which has a functional group having high radical reactivity and can be dissolved or swollen in water or an aqueous alkali solution The plate allows direct recording from digital data using lasers and can maintain excellent performance stability even when exposure and development of an image recording material are performed off-line.

IT **1137-73-1**
RL: MOA (Modifier or additive use); USES (Uses)
(**radical polymerization initiator**; planog. printing plate precursor containing)

RN 1137-73-1 HCAPLUS
CN Glycine, N-(carboxymethyl)-N-phenyl- (9CI) (CA INDEX NAME)



IC ICM B41C001-10
ICS G03F007-033

CC 74-6 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 35, 38

IT 269401-43-6
RL: MOA (Modifier or additive use); USES (Uses)
(**IR-absorber**; vplanog. printing plate precursor containing)

IT 631914-53-9P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(radical **polymerizable** compound; planog. printing plate precursor containing)

IT **1137-73-1**
RL: MOA (Modifier or additive use); USES (Uses)
(**radical polymerization initiator**; planog. printing plate precursor containing)

L128 ANSWER 12 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

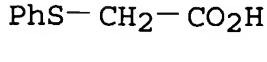
2003:961393 Document No. 140:154288 A Novel Approach to the Preparation of Dissociative Electron Transfer Photoinitiators for Free Radical **Polymerization.** Wrzyszczynski, Andrzej; Pietrzak, Marek; Paczkowski, Jerzy (Faculty of Chemical Technology and Engineering, University of Technology and Agriculture, Bydgoszcz, 85-326, Pol.). Macromolecules, 37(1), 41-44 (English) 2004. CODEN: MAMOBX. ISSN: 0024-9297. Publisher: American Chemical Society.

AB A new approach to the design of the electron transfer free radical photoinitiating system (ETPS) is presented in the paper. The system applying a light absorber (dye), and an electron donor (sulfur-containing aromatic carboxylic acid, SCCA), possessing the structure allowing the formation of the leaving group that forms a neutral free radical, is described. The exptl. results show that after the transformation of the SCCA into its ammonium salt a substantial increase of the **polymerization** photoinitiation ability of the system is observed The mechanism of the photoinitiated **polymerization** for the tested photoredox pairs is clarified on the basis of the laser flash photolysis expts. obtained from the neutral dye (5,7-diiodo-3-pentoxy-6-fluorone, DIPF) serving as electron acceptor and (phenylthio)acetic acid (Ph-S-CH2-COOH, PTAA) and its tetrabutylammonium salt (PTAA AS) as electron donors in MeCN solution It is documented that the photoredn. of DIPF in the presence of (phenylthio)acetic acid and its tetrabutylammonium salt occurs via the photoinduced electron transfer process. On the basis of the known photochem. of sulfur-containing aromatic carboxylic acids, it is postulated that the existence of the carboxyl group in an ionic form allows a rapid **decarboxylation**, yielding a neutral α-alkylthio-type radical (R-S-CH2•). The system described in this paper applies the dissociative electron transfer process for an effective production of very reactive free **radicals** able to **initiate** a **radical polymerization**

IT **103-04-8**, (Phenylthio)acetic acid **122-59-8**
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(preparation of dissociative electron transfer photoinitiators for free radical **polymerization**)

RN 103-04-8 HCAPLUS

CN Acetic acid, (phenylthio)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 122-59-8 HCAPLUS
CN Acetic acid, phenoxy- (8CI, 9CI) (CA INDEX NAME)

PhO—CH_2—CO_2H

CC **74-1** (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 35
ST dissociative electron transfer photoinitiator free radical **polymn** prepn
IT Electron transfer
(photochem.; preparation of dissociative electron transfer photoinitiators for free radical **polymerization**)
IT Photolysis catalysts
Photolysis kinetics
Reduction, photochemical
(preparation of dissociative electron transfer photoinitiators for free radical **polymerization**)
IT **Polymerization**
(radical, kinetics; preparation of dissociative electron transfer photoinitiators for free radical **polymerization**)
IT 36446-02-3, 2-Propenoic acid, 2-ethyl-2-[[(1-oxo-2-propenyl)oxy]methyl]-1,3-propanediyl ester, homopolymer 653593-60-3
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)
(preparation of dissociative electron transfer photoinitiators for free radical **polymerization**)
IT **103-04-8**, (Phenylthio)acetic acid **122-59-8** 7605-25-6 13205-48-6 15625-89-5, 2-Ethyl-2-(hydroxymethyl)-1,3-propanediol triacrylate 16188-55-9 404384-36-7 610769-56-7 653593-61-4 653593-62-5 653593-63-6
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(preparation of dissociative electron transfer photoinitiators for free radical **polymerization**)

L128 ANSWER 13 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
2003:888408 Document No. 140:236163 Preparation of polyesteramides based on aliphatic amine-containing phenol derivatives via interfacial **polymerization**. Kim, Byung-hoon; Lee,

Chil-won; Gong, Myoung-seon (Department of Chemistry, Dankook University, Chungnam, 330-714, S. Korea). Macromolecular Research, 11(5), 328-333 (English) 2003. CODEN: MRAECT. ISSN: 1598-5032. Publisher: Polymer Society of Korea.

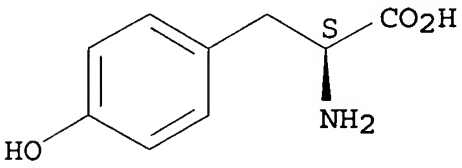
AB A series of poly(ester amides) with a randomly introduced ester/amide group ratio of 50/50 were newly synthesized by reacting terephthaloyl chloride, isophthaloyl chloride or sebacoyl chloride with tyramine or tyrosine. The **polymerization** was carried out by interfacial **polymerization** in two-phase solvent systems, which gave various copolymers with moderate mol. wts. in good yields. The chemical structures of the polymers were confirmed by 1H NMR and **IR** spectra and elemental anal. Tyrosine-based polymers were **decarboxylated** at around 290°C to give the product which was obtainable from tyramine. Thermal stability and degradation behavior were examined by differential scanning calorimetry and thermogravimetric analyses.

IT **60-18-4**, Tyrosine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(model compound starting material; preparation of poly(ester amides)
based on aminoethyl phenol derivs.)

RN 60-18-4 HCAPLUS

CN L-Tyrosine (9CI) (CA INDEX NAME)

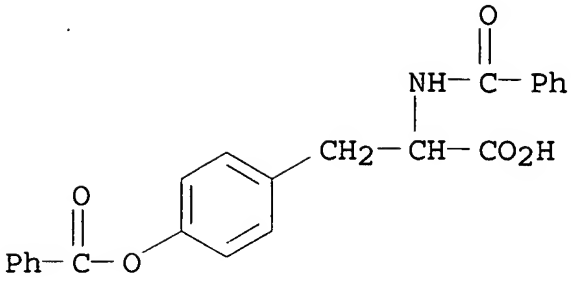
Absolute stereochemistry. Rotation (-).



IT **97485-13-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(model compound; preparation of poly(ester amides) based on aminoethyl
phenol derivs.)

RN 97485-13-7 HCAPLUS

CN Tyrosine, N-benzoyl-, benzoate (ester) (9CI) (CA INDEX NAME)



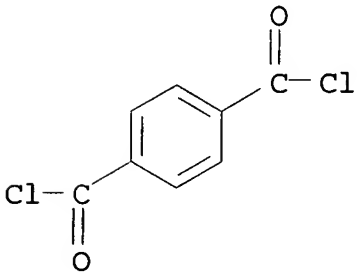
IT **503066-77-1P**, Terephthaloyl chloride-tyrosine copolymer
667871-91-2P, Isophthaloyl chloride-tyrosine copolymer
667871-92-3P, Sebacoyl chloride-tyrosine copolymer
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of poly(ester amides) based on aminoethyl phenol derivs.)

RN 503066-77-1 HCAPLUS

CN L-Tyrosine, polymer with 1,4-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

CM 1

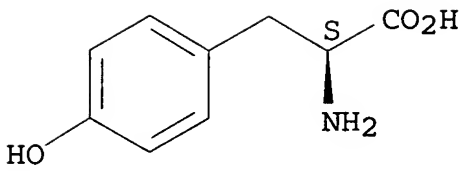
CRN 100-20-9
CMF C8 H4 Cl2 O2



CM 2

CRN 60-18-4
CMF C9 H11 N O3

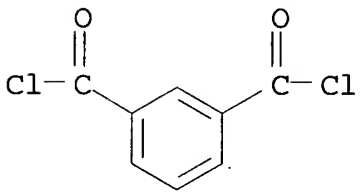
Absolute stereochemistry. Rotation (-).



RN 667871-91-2 HCAPLUS
CN L-Tyrosine, polymer with 1,3-benzenedicarbonyl dichloride (9CI) (CA INDEX NAME)

CM 1

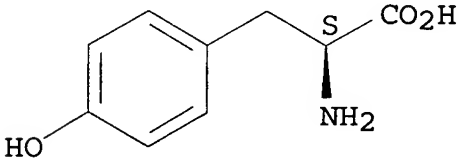
CRN 99-63-8
CMF C8 H4 Cl2 O2



CM 2

CRN 60-18-4
CMF C9 H11 N O3

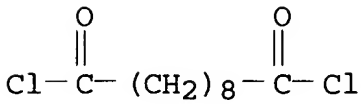
Absolute stereochemistry. Rotation (-).



RN 667871-92-3 HCAPLUS
CN L-Tyrosine, polymer with decanedioyl dichloride (9CI) (CA INDEX NAME)

CM 1

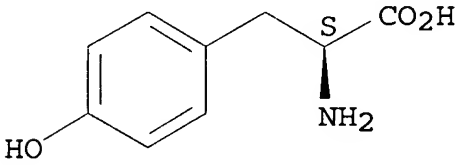
CRN 111-19-3
CMF C10 H16 Cl2 O2



CM 2

CRN 60-18-4
CMF C9 H11 N O3

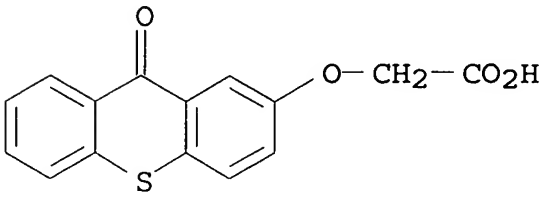
Absolute stereochemistry. Rotation (-).



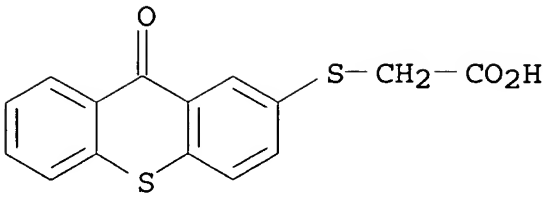
CC 35-5 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 25
IT 51-67-2, Tyramine **60-18-4**, Tyrosine, reactions 98-88-4, Benzoyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(model compound starting material; preparation of poly(ester amides)
based on aminoethyl phenol derivs.)
IT 41859-53-4P **97485-13-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(model compound; preparation of poly(ester amides) based on aminoethyl
phenol derivs.)
IT 232262-40-7P, Isophthaloyl chloride-tyramine copolymer
503066-77-1P, Terephthaloyl chloride-tyrosine copolymer
667871-89-8P, Terephthaloyl chloride-tyramine copolymer
667871-90-1P, Sebacoyl chloride-tyramine copolymer
667871-91-2P, Isophthaloyl chloride-tyrosine copolymer

667871-92-3P, Sebacoyl chloride-tyrosine copolymer
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of poly(ester amides) based on aminoethyl phenol derivs.)

L128 ANSWER 14 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
2003:718628 Document No. 139:365280 One-component bimolecular photoinitiating systems, 2 thioxanthone acetic acid derivatives as photoinitiators for free radical **polymerization.** Aydin, Meral; Arsu, Nergis; Yagci, Yusuf (Department of Chemistry, Yildiz Technical University, Istanbul, 34210, Turk.). Macromolecular Rapid Communications, 24(12), 718-723 (English) 2003. CODEN: MRCOE3. ISSN: 1022-1336. Publisher: Wiley-VCH Verlag GmbH & Co. KGaA.
AB The compds. 2-thioxanthonethioacetic acid and 2-(carboxymethoxy)thioxanthone, bimol. photoinitiators for free radical **polymerization**, are synthesized and characterized. Their capability to act as initiators for the **polymerization** of Me methacrylate is examined The postulated mechanism is based on the intermol. electron-transfer reaction of the excited photoinitiator with the sulfur or oxygen atom of the ground state of the resp. photoinitiator followed by **decarboxylation.** The resulting alkyl **radicals initiate** the **polymerization**
IT **84434-05-9P**, 2-(Carboxymethoxy)thioxanthone
620170-13-0P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of thioxanthone acetic acid derivs. as photoinitiators for radical **polymerization**)
RN 84434-05-9 HCAPLUS
CN Acetic acid, [(9-oxo-9H-thioxanthen-2-yl)oxy]- (9CI) (CA INDEX NAME)



RN 620170-13-0 HCAPLUS
CN Acetic acid, [(9-oxo-9H-thioxanthen-2-yl)thio]- (9CI) (CA INDEX NAME)



IT **103-04-8**, Thiophenoxyacetic acid **122-59-8**,
Phenoxyacetic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of thioxanthone acetic acid derivs. as
photoinitiators for radical **polymerization**)
RN 103-04-8 HCAPLUS
CN Acetic acid, (phenylthio)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

PhS— CH_2— CO_2H

RN 122-59-8 HCAPLUS
CN Acetic acid, phenoxy- (8CI, 9CI) (CA INDEX NAME)

PhO— CH_2— CO_2H

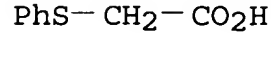
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 27
IT **Polymerization** catalysts
(photochem., radical; preparation of thioxanthone acetic acid derivs.
as photoinitiators for **polymerization** of Me methacrylate)
IT 105-59-9, N-Methyldiethanolamine
RL: CAT (Catalyst use); USES (Uses)
(in catalysts containing thioxanthone acetic acid derivs. for
polymerization of Me methacrylate)
IT **84434-05-9P**, 2-(Carboxymethoxy)thioxanthone
620170-13-0P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP
(Preparation); USES (Uses)
(preparation of thioxanthone acetic acid derivs. as photoinitiators

for radical **polymerization**)
IT **103-04-8**, Thiophenoxyacetic acid **122-59-8**,
Phenoxyacetic acid 147-93-3, Thiosalicylic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of thioxanthone acetic acid derivs. as
photoinitiators for radical **polymerization**)

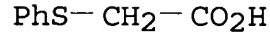
L128 ANSWER 15 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
2002:696833 Document No. 137:352613 Spectral, Kinetics, and Theoretical Studies of Radical Cations Derived from Thioanisole and Its Carboxylic Derivative. Korzeniowska-Sobczuk, Anna; Hug, Gordon L.; Carmichael, Ian; Bobrowski, Krzysztof (Institute of Nuclear Chemistry and Technology, Warsaw, 03-195, Pol.). Journal of Physical Chemistry A, 106(40), 9251-9260 (English) 2002. CODEN: JPCAFH. ISSN: 1089-5639. Publisher: American Chemical Society.
AB Hydroxyl radicals (•OH) react with thioanisole (Ph-S-CH3) via two competitive addition pathways: with the thioether functionality and
with the aromatic ring. At neutral pH, •OH addition leads to the prompt formation of monomeric sulfur radical cations (Ph-S+•-CH3, addition to the thioether group) and hydroxycyclohexadienyl radicals (Ph•-(OH)-S-CH3, addition to the aromatic ring). The latter radicals subsequently decay into products, which do not include the corresponding radical cations with delocalized pos. charge on the aromatic ring (Ph+•-S-CH3). On the other hand, at low pH, •OH addition, both to the thioether functionality and to the aromatic ring, leads promptly only to Ph-S+•-CH3 radical cations. These observations are rationalized in terms of the highly unstable nature of Ph+•-S-CH3 radical cations (formed via proton-catalyzed water elimination from Ph•-(OH)-S-CH3 radicals) and their rapid conversion into Ph-S+•-CH3 radical cations. Addnl. exptl. support for the instability of radical cations derived from aromatic thioethers with delocalized pos. charge on the aromatic ring has been obtained from the
•OH-induced oxidation studies of phenylthioacetic acid (Ph-S-CH2-COOH). At low pH, Ph-S-CH2-COOH undergoes nearly complete (relative to the available •OH radicals) quant. **decarboxylation**, in contrast to neutral pH, at which the yield of **decarboxylation** accounts for only half of the available •OH radicals. To support our conclusions, quantum mech. calcns. were performed using d. functional theory (DFT) that provided predictions of the electronic structure and optical excitation energies of the Ph-S+•-CH3 radical cations and other

key transients.

IT **103-04-8**, (Phenylthio)acetic acid
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(Spectral, Kinetics, and Theor. Studies of Radical Cations Derived from Thioanisole and Its Carboxylic Derivative)
RN 103-04-8 HCAPLUS
CN Acetic acid, (phenylthio)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **103-04-8D**, (Phenylthio)acetic acid, cyclohexadienyl-type radical addition products to aromatic ring
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(Spectral, Kinetics, and Theor. Studies of Radical Cations Derived from Thioanisole and Its Carboxylic Derivative)
RN 103-04-8 HCAPLUS
CN Acetic acid, (phenylthio)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **474459-13-7**
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
(**decarboxylation**; Spectral, Kinetics, and Theor. Studies of Radical Cations Derived from Thioanisole and Its Carboxylic Derivative)
RN 474459-13-7 HCAPLUS
CN Acetic acid, (phenylthio)-, radical ion(1+) (9CI) (CA INDEX NAME)

CC 22-8 (Physical Organic Chemistry)
Section cross-reference(s): **74**
IT Addition reaction
Decarboxylation

(radiolytic; Spectral, Kinetics, and Theor. Studies of Radical Cations Derived from Thioanisole and Its Carboxylic Derivative)

IT **103-04-8**, (Phenylthio)acetic acid 3352-57-6, Hydroxyl, reactions 12143-45-2
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(Spectral, Kinetics, and Theor. Studies of Radical Cations Derived from Thioanisole and Its Carboxylic Derivative)

IT 100-68-5D, Thioanisole, cyclohexadienyl-type radical addition products to aromatic ring **103-04-8D**, (Phenylthio)acetic acid, cyclohexadienyl-type radical addition products to aromatic ring 3352-57-6D, Hydroxyl, cyclohexadienyl-type radical addition products to aromatic rings 4358-92-3D, cyclohexadienyl-type radical addition products to aromatic ring 12385-13-6D, Atomic hydrogen, cyclohexadienyl-type radical addition products to aromatic rings, properties 25087-44-9, (Phenylthio)methyl 158171-90-5, Thioanisole radical cation
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(Spectral, Kinetics, and Theor. Studies of Radical Cations Derived from Thioanisole and Its Carboxylic Derivative)

IT 474459-12-6 **474459-13-7**
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
(**decarboxylation**; Spectral, Kinetics, and Theor. Studies of Radical Cations Derived from Thioanisole and Its Carboxylic Derivative)

IT 12408-02-5, Hydrogen ion, uses
RL: CAT (Catalyst use); USES (Uses)
(**dehydration** catalyst; Spectral, Kinetics, and Theor. Studies of Radical Cations Derived from Thioanisole and Its Carboxylic Derivative)

L128 ANSWER 16 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
2002:228670 Document No. 136:270620 Lithographic master plates fabricated by development-free direct platemaking. Sakata, Itaru; Kawamura, Koichi (Fuji Photo Film Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 2002086943 A2 20020326, 34 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2000-273397 20000908.

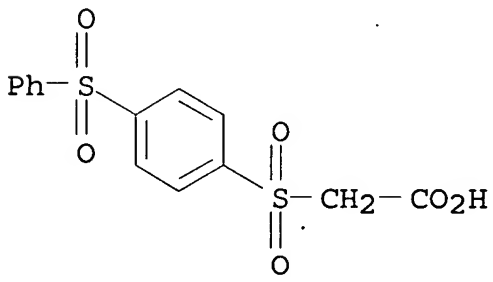
AB The masters, forming clear images without stains in nonimage area, have image-recording layers containing (a) multivalent organic base salts

of R(SO2CH2CO2H)x (R = alkyl, etc.; x = 1, 2) which are thermally **decarboxylated** to release the base moieties (b) hydrophilic macromols. bearing acidic groups reactive to the bases.

IT **97649-40-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(in preparation of organic-base-releasing salts for high-sensitivity lithog. master plates)

RN 97649-40-6 HCAPLUS

CN Acetic acid, [[4-(phenylsulfonyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



IC ICM B41N001-14
ICS G03F007-00; G03F007-004; G03F007-038

CC **74-6** (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 38

ST lithog master thermal **decarboxylation** base precursor; hydrophilic polymer lithog master laser platemaking; latent **crosslinker** thermal **decarboxylation** lithog master

IT Lithographic plates
(high-sensitivity lithog. master plates containing salts showing thermal **decarboxylation** for heat-mode laser direct platemaking)

IT **Crosslinking** agents
(latent; high-sensitivity lithog. master plates containing salts showing thermal **decarboxylation** for heat-mode laser direct platemaking)

IT **97649-40-6** 136168-27-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(in preparation of organic-base-releasing salts for high-sensitivity lithog. master plates)

IT 136168-28-0P

RL: MOA (Modifier or additive use); PNU (Preparation, unclassified); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(latent **crosslinking** agents; high-sensitivity lithog. master plates containing salts showing thermal **decarboxylation** for heat-mode laser direct platemaking)

IT 405096-34-6 405096-36-8 405096-38-0
RL: MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)
(latent **crosslinking** agents; high-sensitivity lithog. master plates containing salts showing thermal **decarboxylation** for heat-mode laser direct platemaking)

IT 9003-01-4DP, Acrylic acid homopolymer, reaction products with methacryloyloxyethyl isocyanate, sodium salt 30674-80-7DP, 2-Methacryloyloxyethyl isocyanate, reaction products with poly(acrylic acid), sodium salt
RL: PNU (Preparation, unclassified); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(recording layers; high-sensitivity lithog. master plates containing salts showing thermal **decarboxylation** for heat-mode laser direct platemaking)

IT 26950-79-8, Methacrylic acid-methyl methacrylate copolymer sodium salt
RL: TEM (Technical or engineered material use); USES (Uses)
(recording layers; high-sensitivity lithog. master plates containing salts showing thermal **decarboxylation** for heat-mode laser direct platemaking)

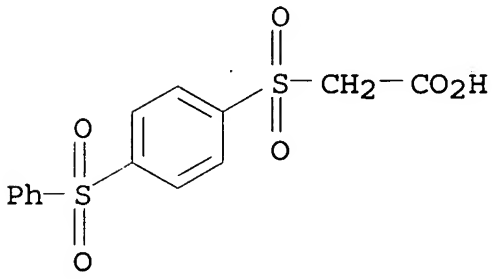
L128 ANSWER 17 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
2000:755235 Document No. 133:342501 Planographic printing plate precursor containing metal compounds, and process for producing planographic printing plates. Kawamura, Koichi (Fuji Photo Film Co., Ltd., Japan). Eur. Pat. Appl. EP 1046496 A1 20001025, 28 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO. (English). CODEN: EPXXDW. APPLICATION: EP 2000-108086 20000425. PRIORITY: JP 1999-113336 19990421; JP 1999-143886 19990524.

AB A planog. printing plate precursor is provided which includes a substrate having thereon an image recording layer containing a metal compound (I-a) which causes a **decarboxylation** reaction by heat and releases a polyvalent metal cation, and a hydrophilic polymer (I-b) which has two or more hydrophilic groups within the same mol. and can coordinate with the polyvalent cation. Also

provided is a planog. printing plate precursor including a substrate having thereon an image recording layer containing a metal complex compound (II-a) and a hydrophilic polymer (II-b) which can coordinate with a metal generated from the metal complex compound by action of heat and which has two or more hydrophilic groups within the mol. and whose main chains are **crosslinked.**

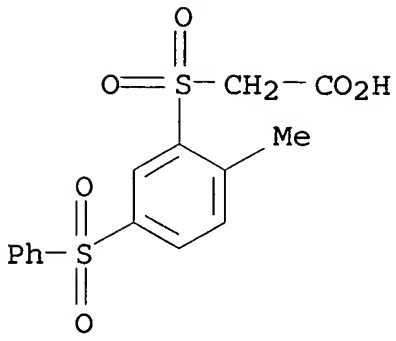
IT **303750-23-4P 303750-24-5P**
RL: PNU (Preparation, unclassified); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(planog. printing plate precursor containing)

RN 303750-23-4 HCAPLUS
CN Acetic acid, [[4-(phenylsulfonyl)phenyl]sulfonyl]-, calcium salt (9CI) (CA INDEX NAME)



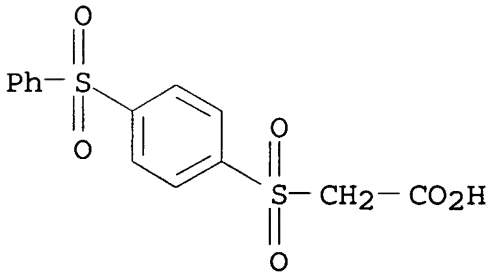
●1/2 Ca

RN 303750-24-5 HCAPLUS
CN Acetic acid, [[2-methyl-5-(phenylsulfonyl)phenyl]sulfonyl]-, calcium salt (9CI) (CA INDEX NAME)

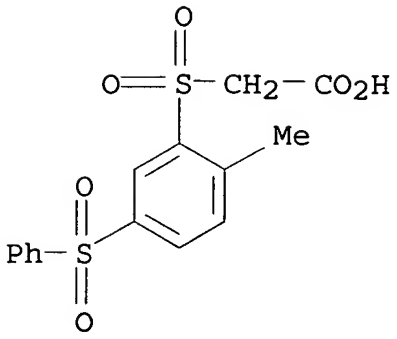


●1/2 Ca

IT **97649-40-6 303750-25-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(planog. printing plate precursor containing)
RN 97649-40-6 HCAPLUS
CN Acetic acid, [[4-(phenylsulfonyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



RN 303750-25-6 HCAPLUS
CN Acetic acid, [[2-methyl-5-(phenylsulfonyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



IC ICM B41C001-10
ICS B41M005-36
CC **74-6** (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
IT 98572-96-4P **303750-23-4P 303750-24-5P**
303751-94-2P
RL: PNU (Preparation, unclassified); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(planog. printing plate precursor containing)
IT 5743-26-0, Calcium acetate monohydrate **97649-40-6**
303750-25-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(planog. printing plate precursor containing)

L128 ANSWER 18 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
2000:387614 Document No. 133:171777 Poly(N-acryl amino acids): A New Class of Biologically Active Polyanions. Bentolila, Alfonso; Vlodavsky, Israel; Ishai-Michaeli, Rivka; Kovalchuk, Olga; Haloun, Christine; Domb, Abraham J. (Department of Medicinal Chemistry School of Pharmacy Faculty of Medicine, The Hebrew University of Jerusalem, Jerusalem, 91120, Israel). Journal of Medicinal Chemistry, 43(13), 2591-2600 (English) 2000. CODEN: JMCMAR. ISSN: 0022-2623. Publisher: American Chemical Society.
AB Poly(N-acryl amino acids) bearing side groups with a lipophilic character or having charged functional groups (i.e. -NH2, -COOH, -SH, -OH, and phenols) were synthesized from the radical **polymerization** of N-acryl amino acid monomers. Monomers were prepared from the reaction of acryloyl chloride and amino acid esters in dry solvents. Polymers of a broad mol. weight ranging from 3 000 to
60 000 Da were obtained. The polymers were optically active, and their structures were confirmed by 1H NMR and **IR** spectra

and elemental anal. Hydroxyl-containing polymers were sulfated in high conversion yields by SO3/pyridine complex. The newly synthesized linear homopolyanions were tested for heparin-like activities: (i) inhibition of heparanase enzyme, (ii) release of basic fibroblast growth factor (bFGF) from the extracellular matrix (ECM), and (iii) inhibition of smooth muscle cell (SMC) proliferation. Polymers based on tyrosine and leucine were highly active in all three tests (microgram level). Polymers based on phenylalanine, tert-leucine, and proline were active as heparanase inhibitors and FGF release, and polymers of trans-hydroxyproline, glycine, and serine were active only as heparanase inhibitors. The polymer of cis-hydroxyproline was inactive. It was found that a net anionic charge (i.e. carboxylic acid) is essential for biol. activity. Thus, Me ester derivs. of the active polymers, zwitterionic amino acid pendent groups (lysine, histidine), and **decarboxylated** amino acids (tyramine, ethanolamine) were inactive. The above active polymers did not exhibit anticoagulation activity which is considered the main limitation of heparin and heparinomimetics for clin. use. These synthetic poly(N-acryl amino acids) may have potential use in the inhibition of heparanase-mediated degradation of basement membranes associated with tumor metastasis, inflammation, and autoimmunity.

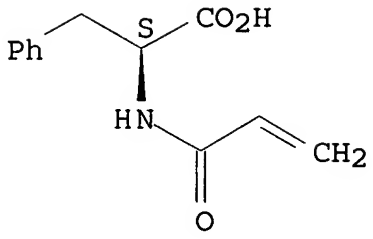
IT **112889-33-5P 192705-89-8P 288325-20-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and structure-activity relations of poly(N-acryl amino acids))

RN 112889-33-5 HCAPLUS
CN L-Phenylalanine, N-(1-oxo-2-propenyl)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 16069-16-2
CMF C12 H13 N O3

Absolute stereochemistry.

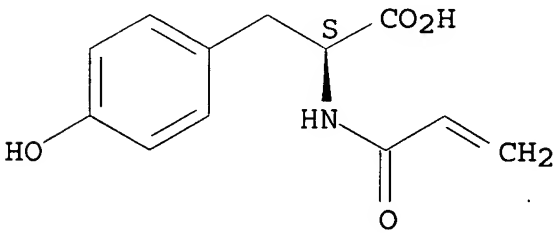


RN 192705-89-8 HCAPLUS
CN L-Tyrosine, N-(1-oxo-2-propenyl)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 192705-88-7
CMF C12 H13 N O4

Absolute stereochemistry.

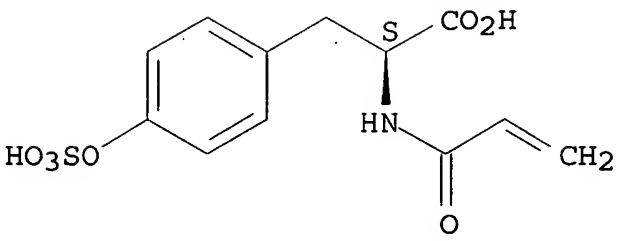


RN 288325-20-2 HCAPLUS
CN L-Tyrosine, N-(1-oxo-2-propenyl)-O-sulfo-, hydrogen sulfate (ester), homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 288325-19-9
CMF C12 H13 N O7 S

Absolute stereochemistry.



CC 1-3 (Pharmacology)
Section cross-reference(s): 34

IT 18939-41-8P 24599-25-5P 28156-60-7P 59809-33-5P 60460-30-2P, L-Proline, 1-(1-oxo-2-propenyl)- 80633-45-0P **112889-33-5P** 125658-47-1P 133287-21-5P 177219-82-8P 186349-23-5P 192705-82-1P **192705-89-8P** 192705-91-2P 192705-92-3P 288325-01-9P 288325-02-0P 288325-03-1P 288325-04-2P 288325-05-3P 288325-06-4P 288325-07-5P 288325-08-6P 288325-09-7P 288325-10-0P 288325-12-2P 288325-14-4P 288325-16-6P 288325-18-8P **288325-20-2P** 288325-22-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and structure-activity relations of poly(N-acryl amino acids))

L128 ANSWER 19 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN.
2000:274574 Document No. 132:315865 Manufacture of lithographic printing plate and photosensitive resin composition. Yamazaki, Sumiaki; Sorori, Tadahiro (Fuji Photo Film Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 2000122272 A2 20000428, 31 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1999-228618 19990812. PRIORITY: JP 1998-229783 19980814.

AB The title process comprises exposing a presensitized lithog. original plate, possessing a recording layer containing a polymer having CO2H and/or its salt groups in which **decarboxylation** occurs by heating and a light-heat converting agent on a support, with **IR** ray lasers to form images. In the process, a lithog. original plate comprising a support coated with a recording layer containing the polymer may be imaged by using a thermal head. The photosensitive resin composition contains a polymer PLXCR1R2CO2H and/or

PLXCR1R2CO2-M+ (X is selected from the groups IV to VI elements and their oxides, sulfides, Se compds, and Te compds.; P = polymer back bone; L = divalent linking group; R1, R2 = univalent group; M = alkali metal, alkaline earth metal, onium), in which **decarboxylation** occurs by heating, and a light-heat converting agent. The lithog. original plates are capable of writing by heat mode exposure with lower energy and shows good storage stability and the resulting printing plates exhibit high printing durability.

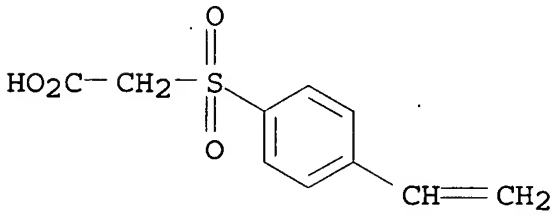
IT **103945-08-0P 122016-80-2P 142180-46-9P 265316-30-1P 265316-33-4P 265316-36-7P 265316-41-4P 265316-44-7P 265316-46-9P 265316-48-1P 265316-50-5P 265316-52-7P 265316-54-9P 265316-56-1P 265316-60-7P 265316-62-9P 265316-64-1P 265316-67-4P 265316-69-6P 265316-72-1P 265316-76-5P**

RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(**polymerization** of; presensitized lithog. plate containing polymer with **decarboxylation** group)

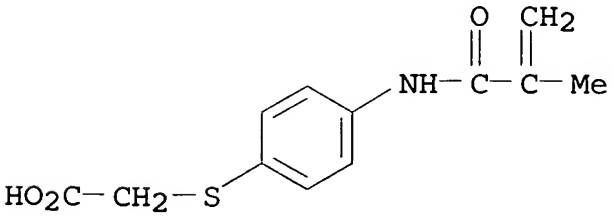
RN 103945-08-0 HCAPLUS

CN Acetic acid, [(4-ethenylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

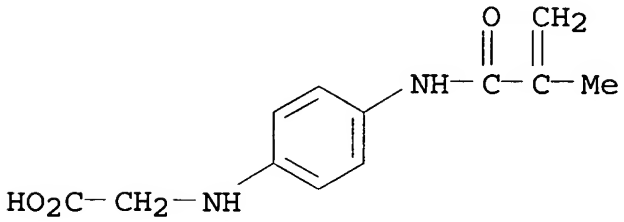


RN 122016-80-2 HCAPLUS

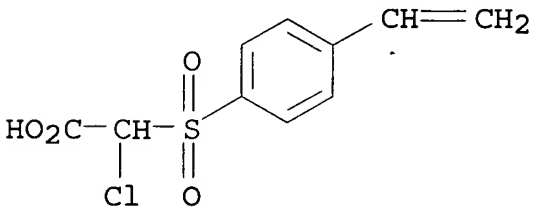
CN Acetic acid, [[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]thio]- (9CI) (CA INDEX NAME)



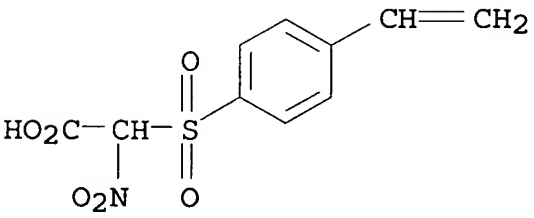
RN 142180-46-9 HCAPLUS
CN Glycine, N-[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]- (9CI) (CA INDEX NAME)



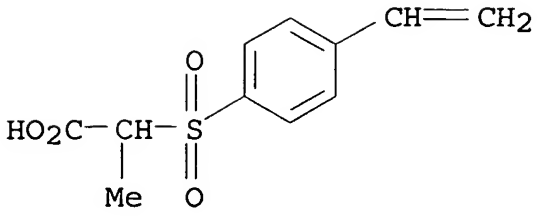
RN 265316-30-1 HCAPLUS
CN Acetic acid, chloro[(4-ethenylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



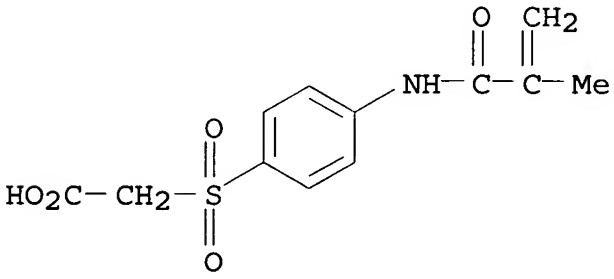
RN 265316-33-4 HCAPLUS
CN Acetic acid, [(4-ethenylphenyl)sulfonyl]nitro- (9CI) (CA INDEX NAME)



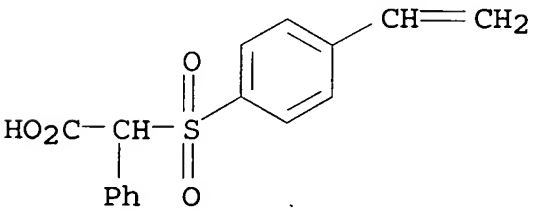
RN 265316-36-7 HCAPLUS
CN Propanoic acid, 2-[(4-ethenylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



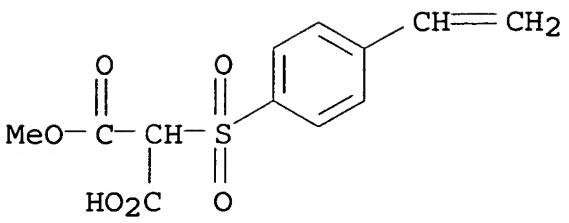
RN 265316-41-4 HCAPLUS
CN Acetic acid, [[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



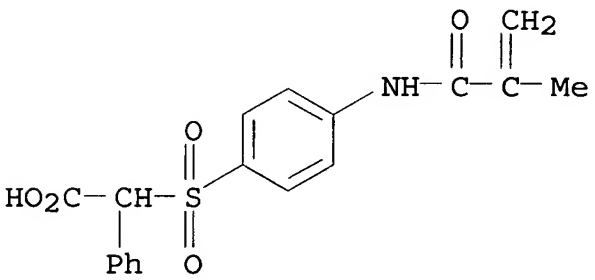
RN 265316-44-7 HCAPLUS
CN Benzeneacetic acid, α-[(4-ethenylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



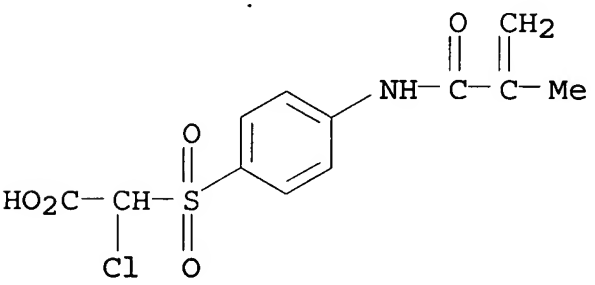
RN 265316-46-9 HCAPLUS
CN Propanedioic acid, [(4-ethenylphenyl)sulfonyl]-, monomethyl ester (9CI) (CA INDEX NAME)



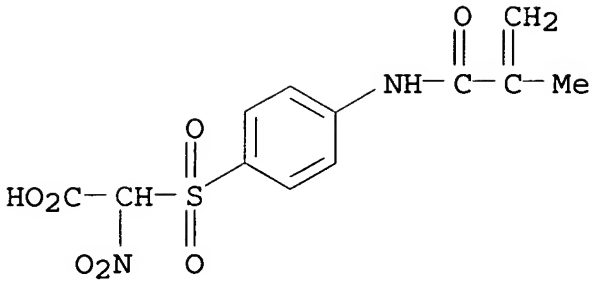
RN 265316-48-1 HCAPLUS
CN Benzeneacetic acid, α-[[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



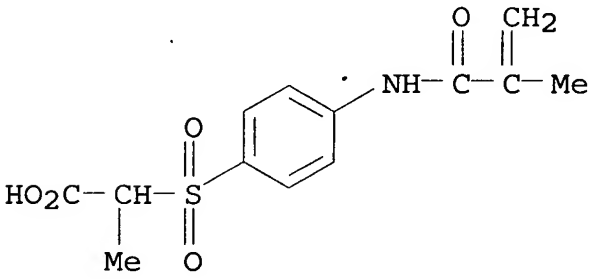
RN 265316-50-5 HCAPLUS
CN Acetic acid, chloro[[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



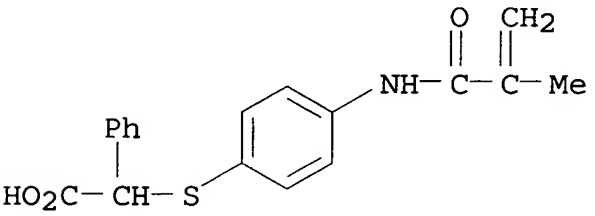
RN 265316-52-7 HCAPLUS
CN Acetic acid, [[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]sulfonyl]nitro- (9CI) (CA INDEX NAME)



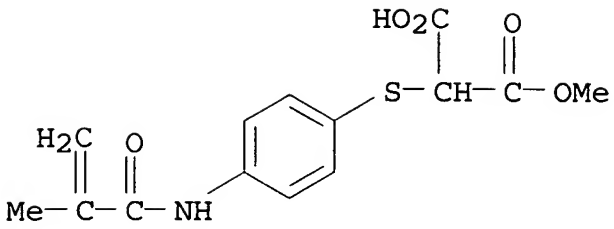
RN 265316-54-9 HCAPLUS
CN Propanoic acid, 2-[[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



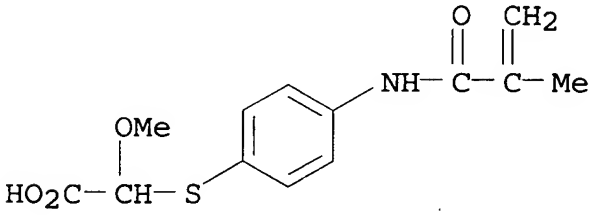
RN 265316-56-1 HCAPLUS
CN Benzeneacetic acid, α-[[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]thio]- (9CI) (CA INDEX NAME)



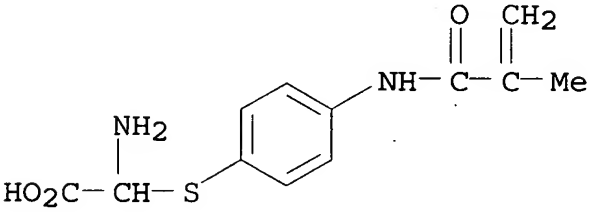
RN 265316-60-7 HCAPLUS
CN Propanedioic acid, [[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]thio]-, monomethyl ester (9CI) (CA INDEX NAME)



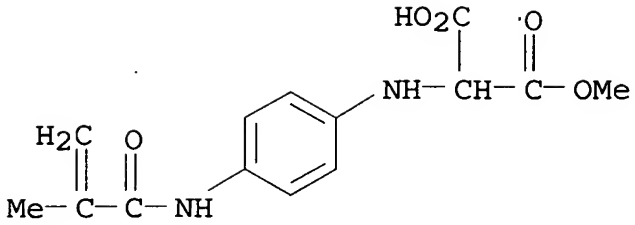
RN 265316-62-9 HCAPLUS
CN Acetic acid, methoxy[[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]thio]- (9CI) (CA INDEX NAME)



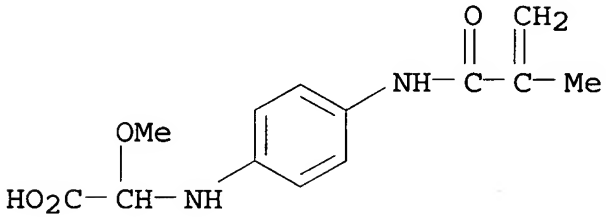
RN 265316-64-1 HCAPLUS
CN Acetic acid, amino[[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]thio]- (9CI) (CA INDEX NAME)



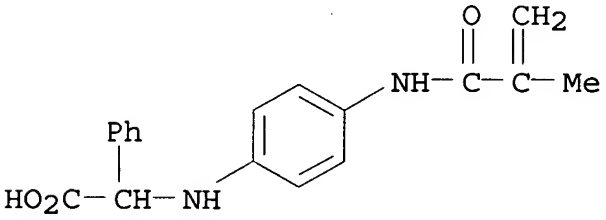
RN 265316-67-4 HCAPLUS
CN Propanedioic acid, [[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]amino]-, monomethyl ester (9CI) (CA INDEX NAME)



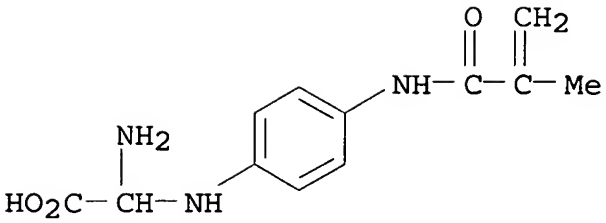
RN 265316-69-6 HCAPLUS
CN Acetic acid, methoxy[[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]amino]- (9CI) (CA INDEX NAME)



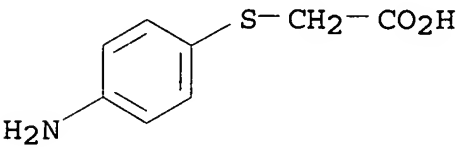
RN 265316-72-1 HCAPLUS
CN Benzeneacetic acid, α-[[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]amino]- (9CI) (CA INDEX NAME)



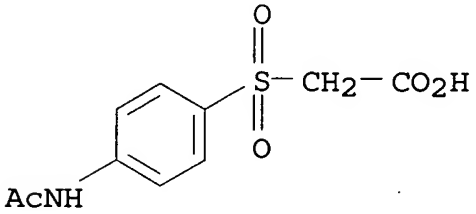
RN 265316-76-5 HCAPLUS
CN Acetic acid, amino[[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]amino]- (9CI) (CA INDEX NAME)



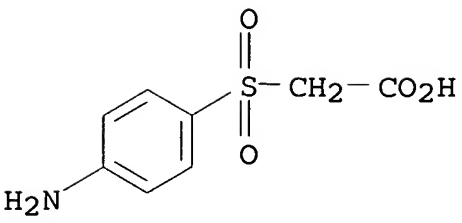
IT **104-18-7P 3406-72-2P 83048-63-9P**
RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation of vinyl monomer with carboxyl group)
RN 104-18-7 HCAPLUS
CN Acetic acid, [(4-aminophenyl)thio]- (9CI) (CA INDEX NAME)



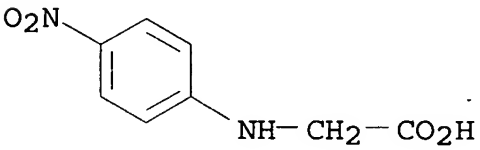
RN 3406-72-2 HCAPLUS
CN Acetic acid, [[4-(acetylamino)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



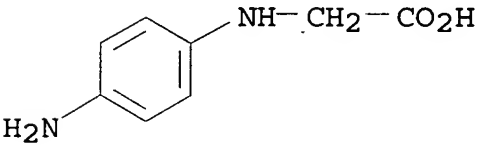
RN 83048-63-9 HCAPLUS
CN Acetic acid, [(4-aminophenyl)sulfonyl]- (9CI) (CA INDEX NAME)



IT **619-91-0 2835-08-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of vinyl monomer with carboxyl group)
RN 619-91-0 HCAPLUS
CN Glycine, N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



RN 2835-08-7 HCAPLUS
CN Glycine, N-(4-aminophenyl)- (9CI) (CA INDEX NAME)



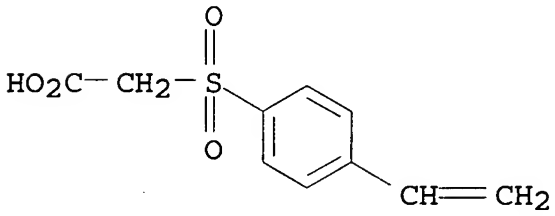
IT **265316-27-6P 265316-31-2P 265316-34-5P**
265316-37-8P 265316-42-5P 265316-43-6P
265316-45-8P 265316-47-0P 265316-49-2P
265316-51-6P 265316-53-8P 265316-55-0P
265316-57-2P 265316-61-8P 265316-63-0P
265316-65-2P 265316-66-3P 265316-68-5P
265316-70-9P 265316-73-2P 265316-77-6P
265316-79-8P 265316-81-2P 265316-90-3P
265316-92-5P 265316-98-1P 265317-10-0P
265317-11-1P 265317-12-2P 265317-15-5P
265317-16-6P 265317-18-8P

RL: DEV (Device component use); PNU (Preparation, unclassified); PREP (Preparation); USES (Uses)
(presensitized lithog. plate containing polymer with **decarboxylation** group)

RN 265316-27-6 HCAPLUS
CN Acetic acid, [(4-ethenylphenyl)sulfonyl]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

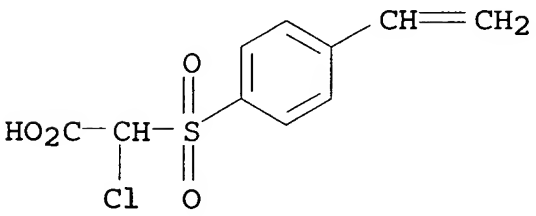
CRN 103945-08-0
CMF C10 H10 O4 S



RN 265316-31-2 HCAPLUS
CN Acetic acid, chloro[(4-ethenylphenyl)sulfonyl]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

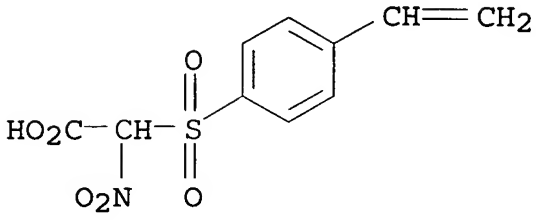
CRN 265316-30-1
CMF C10 H9 Cl O4 S



RN 265316-34-5 HCAPLUS
CN Acetic acid, [(4-ethenylphenyl)sulfonyl]nitro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

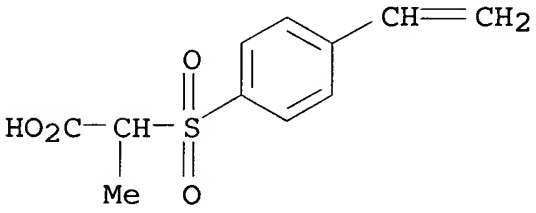
CRN 265316-33-4
CMF C10 H9 N O6 S



RN 265316-37-8 HCAPLUS
CN Propanoic acid, 2-[(4-ethenylphenyl)sulfonyl]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

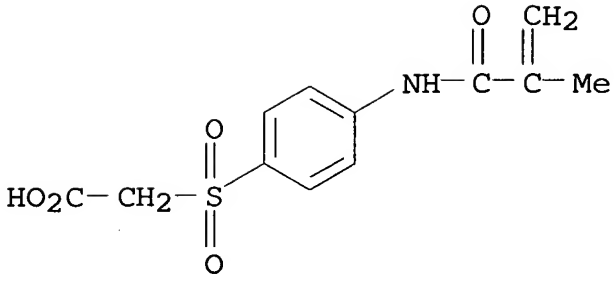
CRN 265316-36-7
CMF C11 H12 O4 S



RN 265316-42-5 HCAPLUS
CN Acetic acid, [[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]sulfonyl]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

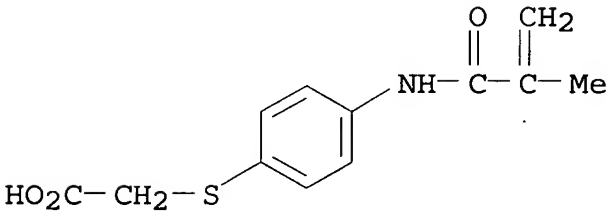
CRN 265316-41-4
CMF C12 H13 N O5 S



RN 265316-43-6 HCAPLUS
CN Acetic acid, [[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]thio]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

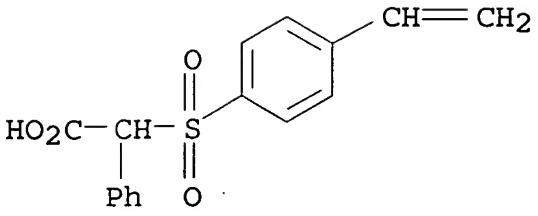
CRN 122016-80-2
CMF C12 H13 N O3 S



RN 265316-45-8 HCAPLUS
CN Benzeneacetic acid, α-[(4-ethenylphenyl)sulfonyl]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

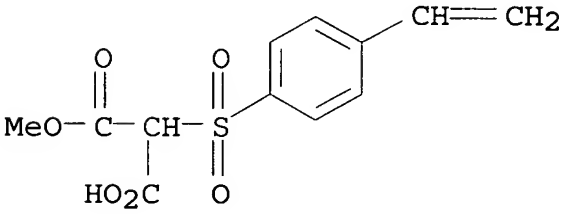
CRN 265316-44-7
CMF C16 H14 O4 S



RN 265316-47-0 HCAPLUS
CN Propanedioic acid, [(4-ethenylphenyl)sulfonyl]-, monomethyl ester, homopolymer (9CI) (CA INDEX NAME)

CM 1

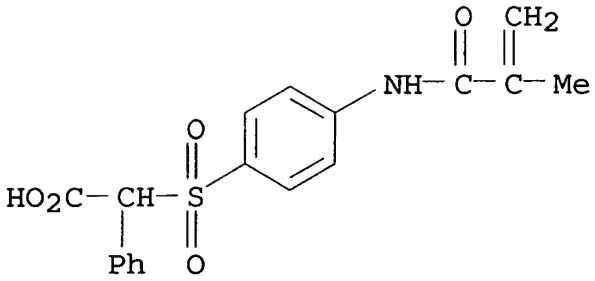
CRN 265316-46-9
CMF C12 H12 O6 S



RN 265316-49-2 HCAPLUS
CN Benzeneacetic acid, α-[[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]sulfonyl]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

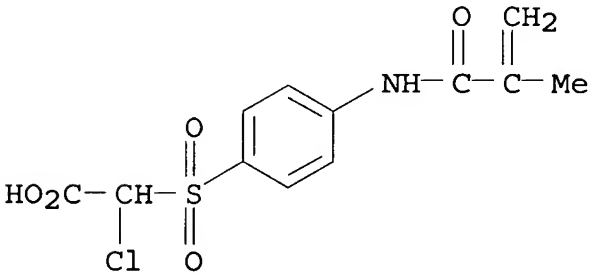
CRN 265316-48-1
CMF C18 H17 N O5 S



RN 265316-51-6 HCAPLUS
CN Acetic acid, chloro[[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]sulfonyl]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

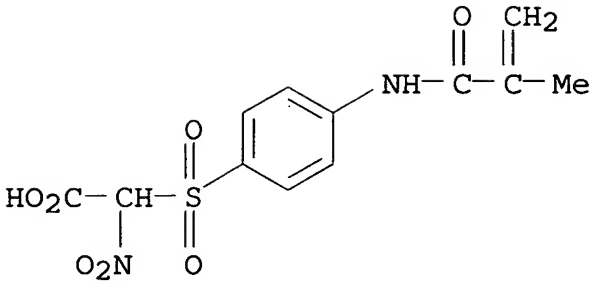
CRN 265316-50-5
CMF C12 H12 Cl N O5 S



RN 265316-53-8 HCAPLUS
CN Acetic acid, [[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]sulfonyl]nitro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

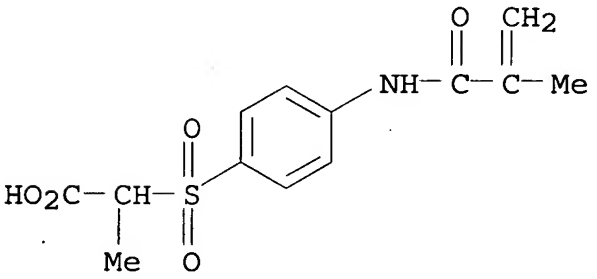
CRN 265316-52-7
CMF C12 H12 N2 O7 S



RN 265316-55-0 HCAPLUS
CN Propanoic acid, 2-[[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]sulfonyl]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

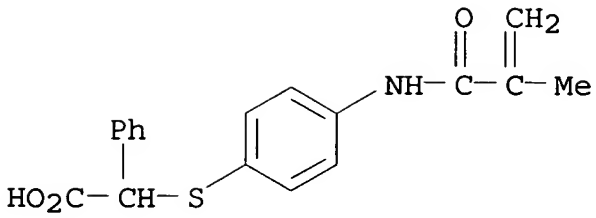
CRN 265316-54-9
CMF C13 H15 N O5 S



RN 265316-57-2 HCAPLUS
CN Benzeneacetic acid, α-[[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]thio]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

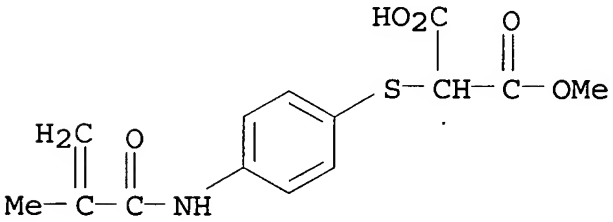
CRN 265316-56-1
CMF C18 H17 N O3 S



RN 265316-61-8 HCAPLUS
CN Propanedioic acid, [[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]thio]-, monomethyl ester, homopolymer (9CI) (CA INDEX NAME)

CM 1

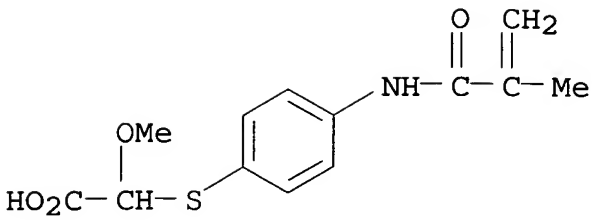
CRN 265316-60-7
CMF C14 H15 N O5 S



RN 265316-63-0 HCAPLUS
CN Acetic acid, methoxy[[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]thio]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

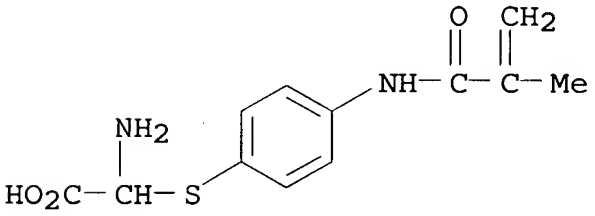
CRN 265316-62-9
CMF C13 H15 N O4 S



RN 265316-65-2 HCAPLUS
CN Acetic acid, amino[[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]thio]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

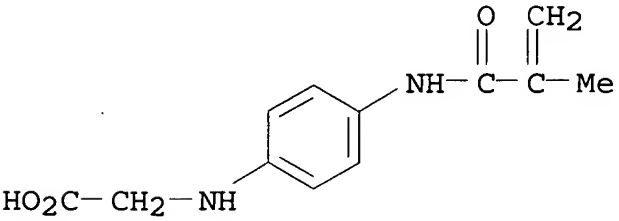
CRN 265316-64-1
CMF C12 H14 N2 O3 S



RN 265316-66-3 HCAPLUS
CN Glycine, N-[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

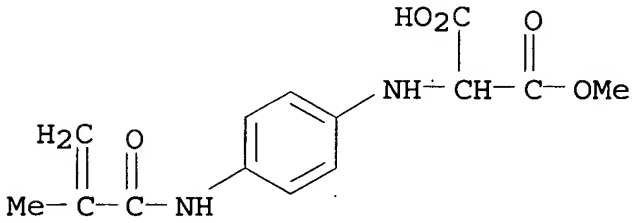
CRN 142180-46-9
CMF C12 H14 N2 O3



RN 265316-68-5 HCAPLUS
CN Propanedioic acid, [[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]amino]-, monomethyl ester, homopolymer (9CI) (CA INDEX NAME)

CM 1

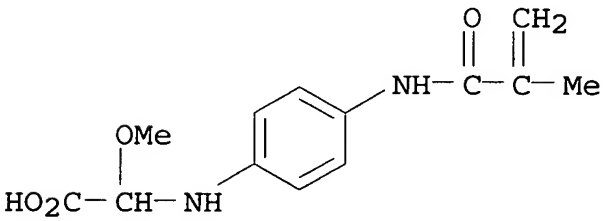
CRN 265316-67-4
CMF C14 H16 N2 O5



RN 265316-70-9 HCAPLUS
CN Acetic acid, methoxy[[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]amino]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

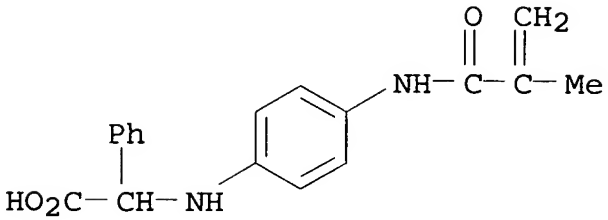
CRN 265316-69-6
CMF C13 H16 N2 O4



RN 265316-73-2 HCAPLUS
CN Benzeneacetic acid, α-[[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]amino]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

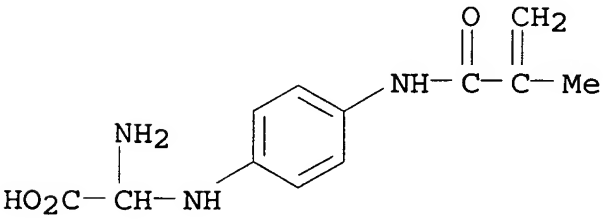
CRN 265316-72-1
CMF C18 H18 N2 O3



RN 265316-77-6 HCAPLUS
CN Acetic acid, amino[[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]amino]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

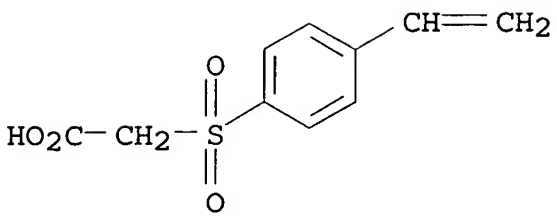
CRN 265316-76-5
CMF C12 H15 N3 O3



RN 265316-79-8 HCAPLUS
CN Acetic acid, [(4-ethenylphenyl)sulfonyl]-, sodium salt, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 265316-78-7
CMF C10 H10 O4 S . Na

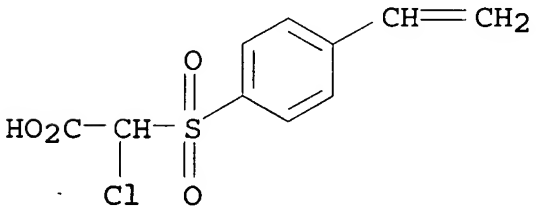


● Na

RN 265316-81-2 HCAPLUS
CN Acetic acid, chloro[(4-ethenylphenyl)sulfonyl]-, potassium salt, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 265316-80-1
CMF C10 H9 Cl O4 S . K

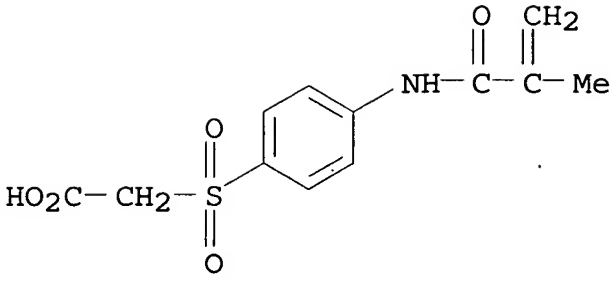


● K

RN 265316-90-3 HCAPLUS
CN Acetic acid, [[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]sulfonyl]-, monosodium salt, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 265316-89-0
CMF C12 H13 N O5 S . Na

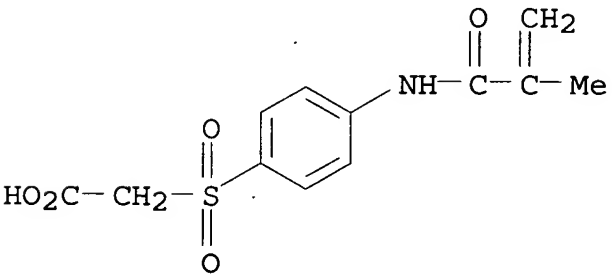


● Na

RN 265316-92-5 HCAPLUS
CN Acetic acid, [[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]sulfonyl]-, monopotassium salt, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 265316-91-4
CMF C12 H13 N O5 S . K

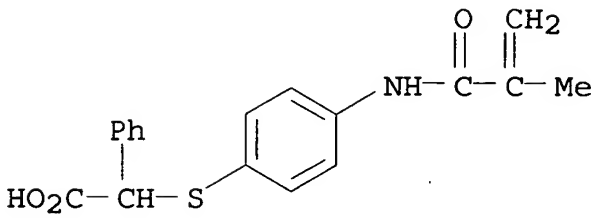


● K

RN 265316-98-1 HCAPLUS
CN Benzeneacetic acid, α-[[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]thio]-, monosodium salt, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 265316-97-0
CMF C18 H17 N O3 S . Na

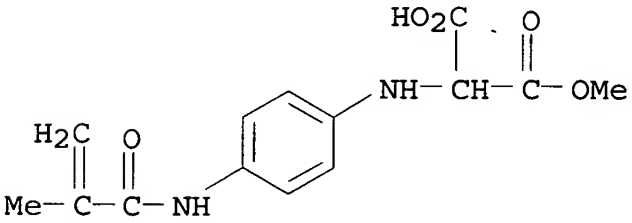


● Na

RN 265317-10-0 HCAPLUS
CN Propanedioic acid, [[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]amino]-, monomethyl ester, monosodium salt, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 265317-09-7
CMF C14 H16 N2 O5 . Na

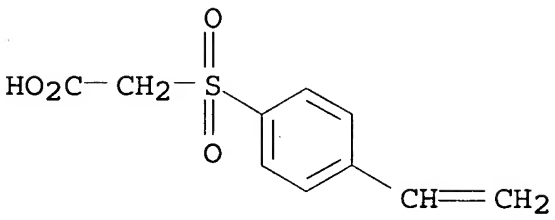


● Na

RN 265317-11-1 HCAPLUS
CN Acetic acid, [(4-ethenylphenyl)sulfonyl]-, polymer with 2-(4-ethenylphenoxy)ethanol (9CI) (CA INDEX NAME)

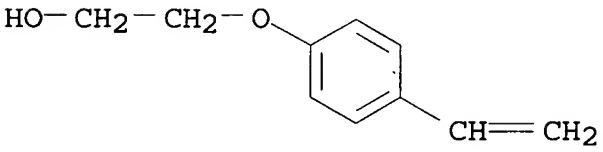
CM 1

CRN 103945-08-0
CMF C10 H10 O4 S



CM 2

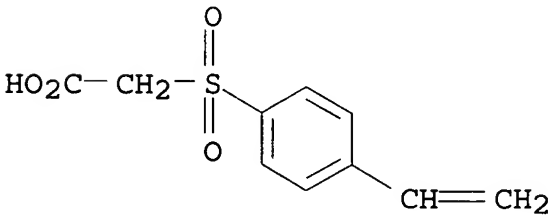
CRN 67521-22-6
CMF C10 H12 O2



RN 265317-12-2 HCAPLUS
CN Benzoic acid, 4-ethenyl-, methyl ester, polymer with [(4-ethenylphenyl)sulfonyl]acetic acid (9CI) (CA INDEX NAME)

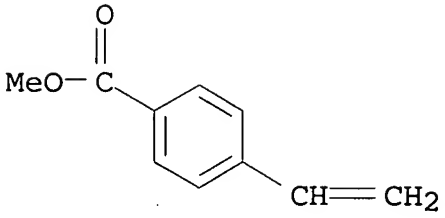
CM 1

CRN 103945-08-0
CMF C10 H10 O4 S



CM 2

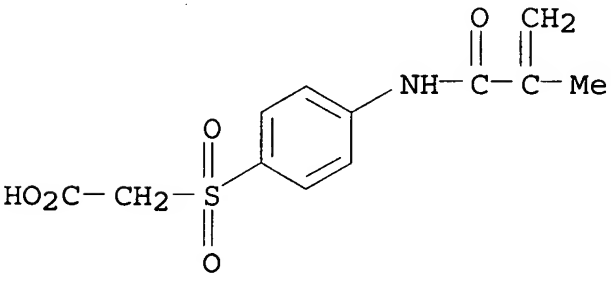
CRN 1076-96-6
CMF C10 H10 O2



RN 265317-15-5 HCAPLUS
CN 2-Propenoic acid, 2-methyl-, 2-hydroxyethyl ester, polymer with [[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]sulfonyl]acetic acid (9CI) (CA INDEX NAME)

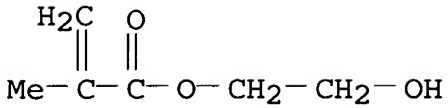
CM 1

CRN 265316-41-4
CMF C12 H13 N O5 S



CM 2

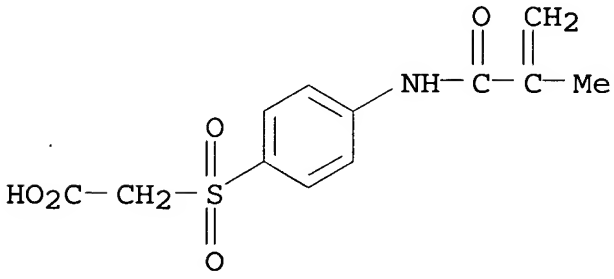
CRN 868-77-9
CMF C6 H10 O3



RN 265317-16-6 HCAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with [[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]sulfonyl]acetic acid (9CI) (CA INDEX NAME)

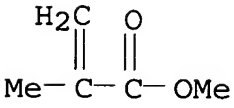
CM 1

CRN 265316-41-4
CMF C12 H13 N O5 S



CM 2

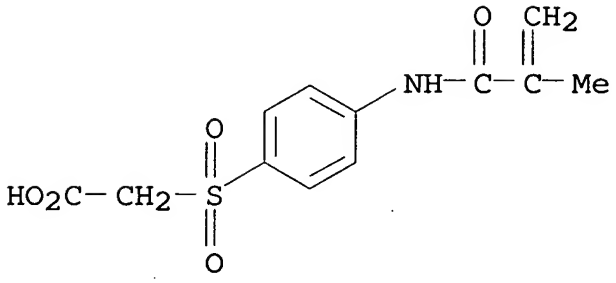
CRN 80-62-6
CMF C5 H8 O2



RN 265317-18-8 HCAPLUS
CN 2-Propenoic acid, 2-methyl-, ethyl ester, polymer with [[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]sulfonyl]acetic acid (9CI) (CA INDEX NAME)

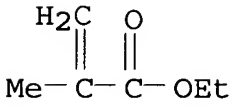
CM 1

CRN 265316-41-4
CMF C12 H13 N O5 S



CM 2

CRN 97-63-2
CMF C6 H10 O2



IC ICM G03F007-00
ICS B41N001-14; G03F007-004; G03F007-038
CC **74-6** (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 38
ST presensitized lithog plate polymer **decarboxylation**; light heat converting agent lithog plate
IT Lithographic plates
(presensitized; presensitized lithog. plate containing polymer with **decarboxylation** group)
IT 22371-56-8P, NK 3508
RL: DEV (Device component use); PNU (Preparation, unclassified); PREP (Preparation); USES (Uses)
(**IR absorbent**; presensitized lithog. plate containing polymer with **decarboxylation** group)
IT **103945-08-0P 122016-80-2P 142180-46-9P**
265316-30-1P 265316-33-4P 265316-36-7P
265316-39-0P **265316-41-4P 265316-44-7P**

265316-46-9P 265316-48-1P 265316-50-5P
265316-52-7P 265316-54-9P 265316-56-1P
265316-58-3P **265316-60-7P 265316-62-9P**
265316-64-1P 265316-67-4P 265316-69-6P
265316-72-1P 265316-74-3P **265316-76-5P**
RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(**polymerization** of; presensitized lithog. plate containing polymer with **decarboxylation** group)

IT **104-18-7P 3406-72-2P 83048-63-9P**
RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation of vinyl monomer with carboxyl group)

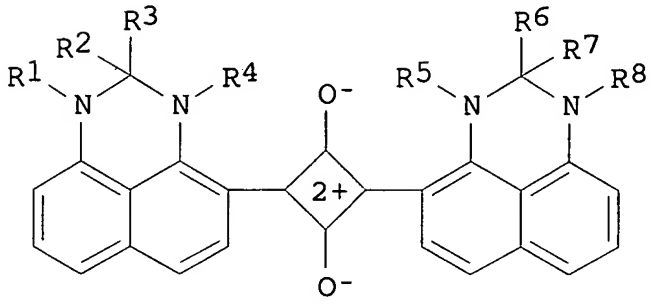
IT 121-60-8, N-Acetylsulfanilyl chloride **619-91-0** 920-46-7, Methacrylic acid chloride 1193-02-8, 4-Aminothiophenol 2633-67-2, p-Styrenesulfonyl chloride **2835-08-7** 3926-62-3, Sodium chloroacetate 212580-45-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of vinyl monomer with carboxyl group)

IT **265316-27-6P 265316-31-2P 265316-34-5P**
265316-37-8P 265316-40-3P **265316-42-5P**
265316-43-6P 265316-45-8P 265316-47-0P
265316-49-2P 265316-51-6P 265316-53-8P
265316-55-0P 265316-57-2P 265316-59-4P
265316-61-8P 265316-63-0P 265316-65-2P
265316-66-3P 265316-68-5P 265316-70-9P
265316-73-2P 265316-75-4P **265316-77-6P**
265316-79-8P 265316-81-2P 265316-83-4P
265316-84-5P 265316-86-7P 265316-88-9P **265316-90-3P**
265316-92-5P 265316-94-7P 265316-95-8P 265316-96-9P
265316-98-1P 265317-00-8P 265317-02-0P 265317-04-2P
265317-06-4P 265317-08-6P **265317-10-0P**
265317-11-1P 265317-12-2P 265317-13-3P
265317-14-4P **265317-15-5P 265317-16-6P**
265317-18-8P 265317-19-9P 265317-21-3P 265317-22-4P
265317-24-6P 265317-25-7P 265317-26-8P 265317-27-9P
265317-28-0P
RL: DEV (Device component use); PNU (Preparation, unclassified); PREP (Preparation); USES (Uses)
(presensitized lithog. plate containing polymer with **decarboxylation** group)

L128 ANSWER 20 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1998:277339 Document No. 129:10697 Laser-induced heat mode recording material containing dihydroxyperimidine squarilium dyes. Ishihara,

Shin; Harada, Toru (Fuji Photo Film Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 10114151 A2 19980506 Heisei, 23 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1996-272282 19961015.

GI



I

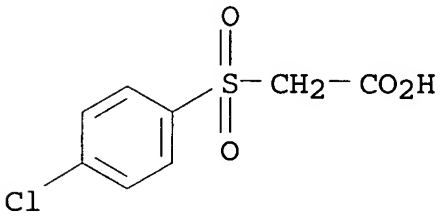
AB In a heat mode recording material including imagewise-heating step using laser having ≥700 nm luminescence, the recording material possesses on a support, at least one thermal recording layer containing a substance of formula LD.HA (LD = colorless or light colored leuco dye; HA = an acid which looses its acidity due to decomposition or evaporation upon heating; LD.HA represents the colored form of LD colored by HA) discoloring on heating, and said thermal recording layer or other layer containing said thermal recording layer contains a **IR absorbing** substance selected from a cyanine dye possessing ClO4- counter ions and a dihydroxyperimidine squarilium dye (I; R1 - R8 = H, alkyl, cycloalkyl, aryl; R1 and R2, R3 and R4 , R5 and R6, R7 and R8, R2 and R3 and/or R6 and R7 are bonded together to form a 5- or 6-membered ring). HA is a carboxylic acid which undergoes **decarboxylation** upon heating and LD is a leuco dye which undergoes coloration upon ring cleavage by an acid. The recording material possesses a back layer across the support opposite to the image-forming layer, and degree of smoothness of the outer most surface of the back layer is ≤4,000 s. It also possesses an overcoat layer containing tetrafluoroethylene beads but not containing a substance discoloring upon heating which is located further away from the support than the thermal recording layer. This recording material gives stable images without installation of a large-scale collector for removed substances and enables single-heat mode recording. Use of the **IR-absorbing** dyes I

markedly improves Dmin and the overcoat layer provides large matting effect on images and makes reading easy by covering finger print marks.

IT **3405-89-8**
RL: TEM (Technical or engineered material use); USES (Uses)
(laser-induced heat mode recording material containing dihydroxyperimidine squarilium dyes)

RN 3405-89-8 HCAPLUS

CN Acetic acid, [(4-chlorophenyl)sulfonyl]- (9CI) (CA INDEX NAME)



IC ICM B41M005-26
ICS B41M005-36

CC 74-12 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

ST laser induced heat mode recording material; hydroxyperimidine squarilium dye **IR absorbing**

IT Dyes
(**IR-absorbing**; laser-induced heat mode recording material containing dihydroxyperimidine squarilium dyes)

IT **3405-89-8** 95235-29-3 110992-72-8 190544-02-6 201024-57-9 206564-80-9 207351-77-7 207351-78-8 207351-79-9
RL: TEM (Technical or engineered material use); USES (Uses)
(laser-induced heat mode recording material containing dihydroxyperimidine squarilium dyes)

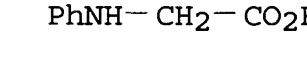
L128 ANSWER 21 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

1997:374006 Document No. 127:128593 Preparation and photoreaction of two-component molecular crystals between aza-aromatic compounds and N-phenylglycine. Koshima, Hideko; Ding, Kuiling; Miura, Takashi; Matsuura, Teruo (PRESTO, Research Development Research Corporation of Japan, Faculty of Science and Technology, Ryukoku University, Seta, Otsu, 520, Japan). Journal of Photochemistry and Photobiology, A: Chemistry, 104(1-3), 105-112 (English) 1997. CODEN: JPPCEJ. ISSN: 1010-6030. Publisher: Elsevier.

AB Crystalline 1:1 two-component mol. compds. ("two-component mol. crystals") crystallized from a solution of a mixture of an aza-aromatic compound

(acridine or phenanthridine) and N-phenylglycine. These two-component mol. crystals were characterized by various phys. methods, including X-ray crystallog. anal. UV irradiation of the crystals was carried out in the solid and solution phases to give aniline, N-methylaniline, formanilide and **decarboxylating** condensation products. The product ratio was dependent on the reaction conditions. Particular attention is focused on the selectivity of the photoreactions in the solid state compared with those in the solution phase and the factors controlling the photoreactions.

IT **103-01-5**, N-Phenylglycine
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and photoreaction of two-component mol. crystals between
aza-aromatic compds. and N-phenylglycine)
RN 103-01-5 HCAPLUS
CN Glycine, N-phenyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC **74-1** (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 22
IT Condensation reaction
Decarboxylation
Hydrogen bond
Molecular crystals
Molecular structure
Photolysis
(preparation and photoreaction of two-component mol. crystals between
aza-aromatic compds. and N-phenylglycine)
IT **103-01-5**, N-Phenylglycine 229-87-8, Phenanthridine 260-94-6, Acridine
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and photoreaction of two-component mol. crystals between
aza-aromatic compds. and N-phenylglycine)

L128 ANSWER 22 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1996:581742 Document No. 125:342526 Photoredox reactions of ArXCOOH (X = CH2, OCH2, SCH2, SOCH2, or SO2CH2) on TiO2. Somasundaram, N.; Srinivasan, C. (Dep. Materials Science, Madurai Kamaraj Univ.,

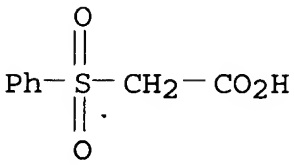
Madurai, 625 021, India). Journal of Photochemistry and Photobiology, A: Chemistry, 99(1), 67-70 (English) 1996. CODEN: JPPCEJ. ISSN: 1010-6030. Publisher: Elsevier.

AB TiO2 acts as a site-selective photocatalyst for sulfur compds. containing S or SO2 and COOH groups in redox reactions. While phenylacetic and phenoxyacetic acids undergo oxidative **decarboxylation** on irradiated TiO2, arylthioacetic acids are oxidized to the corresponding sulfinylacetic acids. Arylsulfonylacetic acids undergo photoinduced reduction with retention of carboxyl group.

IT **3959-23-7**
RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(titania mediated photoredox reactions for site selectivity in multifunctional compds. containing S, SO2, and COOH groups)

RN 3959-23-7 HCAPLUS

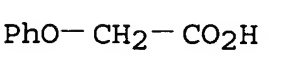
CN Acetic acid, (phenylsulfonyl)- (6CI, 8CI, 9CI) (CA INDEX NAME)



IT **122-59-8**, Phenoxyacetic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(titania mediated photoredox reactions for site selectivity in multifunctional compds. containing S, SO2, and COOH groups)

RN 122-59-8 HCAPLUS

CN Acetic acid, phenoxy- (8CI, 9CI) (CA INDEX NAME)



CC **74-1** (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 67

ST titania photocatalyst site selective photoredox reaction; oxidative photochem **decarboxylation** phenylacetic phenoxyacetic acid; photolysis photooxidn photoredn titania photochem catalyst

IT **Decarboxylation**
(oxidative, photochem., titania mediated photoredox reactions for

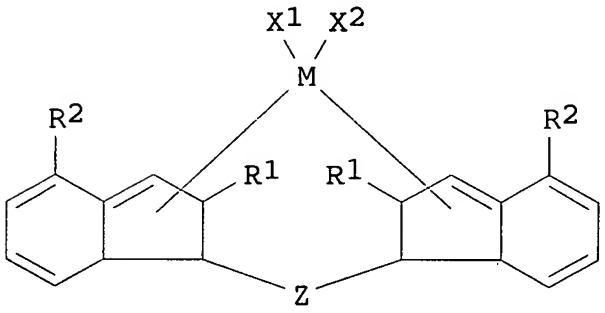
site selectivity in multifunctional compds. containing S, SO2, and COOH groups)

IT 103-04-8, Phenylthioacetic acid 383-38-0 3405-88-7 3405-89-8 3406-73-3 3937-96-0 3937-99-3 3959-08-8 **3959-23-7** 3996-29-0
RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(titania mediated photoredox reactions for site selectivity in multifunctional compds. containing S, SO2, and COOH groups)

IT 103-82-2, Phenylacetic acid, reactions **122-59-8**, Phenoxyacetic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(titania mediated photoredox reactions for site selectivity in multifunctional compds. containing S, SO2, and COOH groups)

L128 ANSWER 23 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1995:928192 Document No. 123:314849 Indenyl transition metal complexes for olefin **polymerization** catalysts. Imuta, Junichi; Fukuoka, Daisuke; Yoshida, Masayasu; Saito, Junji; Fujita, Terunori; Tashiro, Takashi; Kawaai, Koji; Ueda, Takashi; Kiso, Yoshihisa (Mitsui Petrochemical Industries, Ltd., Japan). Can. Pat. Appl. CA 2135561 AA 19950513, 66 pp. (English). CODEN: CPXXEB. APPLICATION: CA 1994-2135561 19941110. PRIORITY: JP 1993-377819 19931112.

GI



I

AB Title complexes I [M = Group IVA, VA, or VIA metal; X1, X2 = H, halo, C1-20 (halogenated) hydrocarbyl, or O- or S-containing group; R1 = C1-20 hydrocarbyl; R2 = halogenated C1-20-hydrocarbyl-substituted C6-16 aryl; Z = (halogenated) C1-20 hydrocarbylene, divalent Si-, Ge-, or Sn-containing group; O, CO, S, SO, SO2, NR3, PR3, P(O)R3, BR3,

or AlR3, R3 = H, halo, or (halogenated) C1-20 hydrocarbyl] are useful as highly active catalysts in the **polymerization** of olefins giving polyolefins having a high m.p. and a high mol. weight

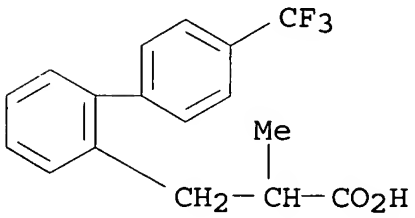
I

are used with organoaluminum cocatalysts or compds. that form ion pairs with I, and the catalysts may be supported on inorg. compds. A typical catalyst was manufactured by lithiation of 2-methyl-4-(p-trifluoromethylphenyl)indene, reaction of the lithiated product with Me2SiCl2, lithiation of the resulting product, and complexation of the 2nd lithiated product with ZrCl2.

IT **167021-53-6P**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(manufacture and chlorination of)

RN 167021-53-6 HCAPLUS

CN [1,1'-Biphenyl]-2-propanoic acid, α-methyl-4'-(trifluoromethyl)- (9CI) (CA INDEX NAME)



IC ICM C07F007-00
ICS C07F009-00; C07F011-00; C08F010-00; C08F004-74; C08F004-622

CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 67

ST indene deriv transition metal complex catalyst; olefin **polymn** catalyst transition metal complex; methyltrifluoromethylphenylindene silylbis metal complex **polymn** catalyst

IT **Polymerization** catalysts
(indenyl transition metal complexes for olefin **polymerization** catalysts)

IT Group IVA element compounds
Group VA element compounds
Group VIA element compounds
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(indenyl transition metal complexes for olefin **polymerization**

catalysts)
IT Aluminoxanes
RL: CAT (Catalyst use); USES (Uses)
(Me, cocatalyst; indenyl transition metal complexes for olefin **polymerization** catalysts)
IT Alkenes, preparation
RL: IMF (Industrial manufacture); PREP (Preparation)
(polymers, indenyl transition metal complexes for olefin **polymerization** catalysts)
IT 167021-58-1P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(catalyst precursor; indenyl transition metal complexes for olefin **polymerization** catalysts)
IT 100-99-2, Triisobutylaluminum, uses 1109-15-5, Tris(pentafluorophenyl)boron
RL: CAT (Catalyst use); USES (Uses)
(cocatalyst; indenyl transition metal complexes for olefin **polymerization** catalysts)
IT 167021-59-2P
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(indenyl transition metal complexes for olefin **polymerization** catalysts)
IT 9003-07-0P, Polypropylene
RL: IMF (Industrial manufacture); PREP (Preparation)
(indenyl transition metal complexes for olefin **polymerization** catalysts)
IT **167021-53-6P**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(manufacture and chlorination of)
IT 167021-52-5P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(manufacture and **decarboxylation** of)
IT 167021-56-9P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(manufacture and **dehydration** of)

L128 ANSWER 24 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1995:42032 Document No. 122:326147 Mechanism for N-phenylglycine-thioxanthene dye photoinitiating system and its application to photopolymer. Naitoh, K.; Shima, M.; Koseki, K.; Yamaoka, T. (Fac.

Eng., Chiba Univ., Chiba, 263, Japan). Chem. Funct. Dyes, Proc. Int. Symp., 2nd, Meeting Date 1992, 632-5. Editor(s): Yoshida, Z.; Shirota, Y. Mita Press: Tokyo, Japan. (English) 1993. CODEN: 59TQAX.

AB Photoinduced processes were studied in the photoinitiator system containing 3-ethoxy-2-phenyl-1H-naphtho(2,1,8-mna)thioxanthe-1-one (TXD) and N-phenylglycine derivative (NPG) quencher. Photolysis study show that quenching of TXD included electron-transfer from ground state of NPG to both the excited singlet and triplet TXD. Radical generation occurred via electron-transfer from ground state NPG to excited TXD, a subsequent **decarboxylation** of NPG radical, and the simultaneous proton transfer from NPG aminium radical. Good laser exposed images were obtained on Al plate using the photosensitive layer containing TXD/NPG initiator.

IT **103-01-5**, N-Phenylglycine
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(mechanism of photoprocesses in phenylglycine-thioxanthene dye photoinitiating system for visible laser photopolymer photoimaging)

RN 103-01-5 HCAPLUS

CN Glycine, N-phenyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

CC **74-1** (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

IT **103-01-5**, N-Phenylglycine 351-95-1 5465-90-7, N-(4-Chlorophenyl)glycine 21911-69-3 22094-69-5 42288-26-6, N-(4-Cyanophenyl)glycine 89101-04-2 102355-72-6, 3-Ethoxy-2-phenyl-1H-naphtho(2,1,8-mna)thioxanthe-1-one
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(mechanism of photoprocesses in phenylglycine-thioxanthene dye photoinitiating system for visible laser photopolymer photoimaging)

L128 ANSWER 25 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

1994:54699 Document No. 120:54699 Metallocenes having benzo-fused indenyl derivatives as ligands, processes for their preparation and their use as olefin **polymerization** catalysts. Rohrmann, Juergen; Dolle, Volker; Winter, Andreas; Kueber, Frank (Hoechst

A.-G., Germany). Can. Pat. Appl. CA 2084017 AA 19930531, 44 pp. (English). CODEN: CPXXEB. APPLICATION: CA 1992-2084017 19921127. PRIORITY: DE 1991-4139595 19911130.

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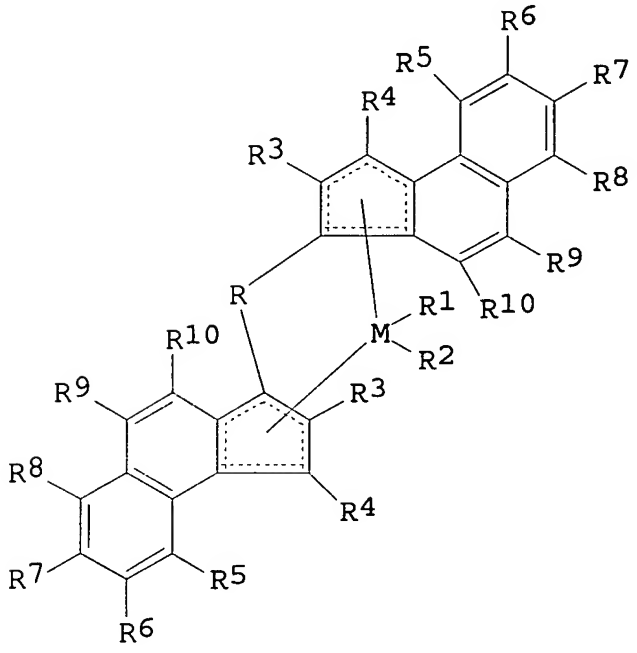

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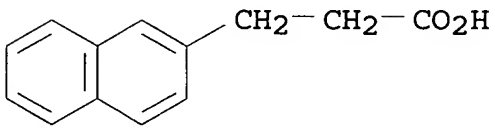
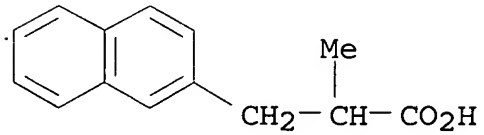
AB Compds. of formula I [M = metal of Group IVB, VB, VIB (preferably Zr or Hf), R1 and R2 are identical or different and may include H, alkyl, alkoxy, aryl, alkenyl, OH or halogen; R3 to R10 are identical or different and may include H, halogen, alkyl, aryl or NR12, SR1, OSiR13, SiR13 or PR12 in which R1 is a halogen atom, an alkyl group or an aryl group; in addition, adjacent radicals R4 to R10, with atoms joining them may form an aromatic or aliphatic ring; R is a (substituted) alkylene or heteroatom bridge, e.g., BR11, AlR11, Ge, Sn, O, S, SO, NR11, CO, PR11 or P(O)R11, in which R11 may be H, halogen, alkyl, fluoroalkyl, etc.] are claimed, along with a process for their preparation The process comprises reacting compound I (wherein MR1R2 = nothing) with MX4, eg.., TiCl4 (M = Ti, X = Cl). I are shown to **polymerize** olefins, e.g., propylene in the presence of

methylaluminoxane.
IT **21658-35-5P**, 2-Naphthalenepropanoic acid
107777-19-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and sequential chlorination and intramol.
Friedel-Crafts
acylation of, benzoindanone derivative from, olefin **polymerization**
catalysts preparation by)
RN 21658-35-5 HCAPLUS
CN 2-Naphthalenepropanoic acid (9CI) (CA INDEX NAME)



RN 107777-19-5 HCAPLUS
CN 2-Naphthalenepropanoic acid, α-methyl- (9CI) (CA INDEX NAME)



IC ICM C07F007-00
ICS C07F009-00; C07F011-00; C08F004-74
CC 29-10 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 25, 35
ST metallocene benzofused indenyl catalyst olefin **polymn**
IT **Polymerization** catalysts
((benzo-fused indenyl)metallocenes, preparation and activity as,
for
propylene)
IT Alkenes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(**polymerization** of, metallocene catalysts for)
IT Aluminoxanes
RL: CAT (Catalyst use); USES (Uses)
(Me, cocatalyst, in the (benzo-fused indenyl)metallocene-
catalyzed **polymerization** of propylene)
IT 115-07-1, 1-Propene, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)
((benzo-fused indenyl)metallocene-catalyzed **polymerization** of)

IT 105-53-3 609-08-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with bromomethylnaphthalene, olefin **polymerization** catalysts preparation by)

IT 939-26-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with methylmalonate, olefin **polymerization** catalysts preparation by)

IT 533-98-2, 1,2-Dibromobutane
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reactions of, with benzoindene derivative, olefin **polymerization** catalysts preparation by)

IT 75-78-5 106-93-4 149-74-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reactions of, with benzoindenyllithium derivs., olefin **polymerization** catalysts preparation by)

IT 10026-11-6, Zirconium tetrachloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reactions of, with silanediylbis(benzoindenyl) derivs., olefin **polymerization** catalysts preparation by)

IT 149237-92-3P 151492-19-2P 151593-48-5P 152071-12-0P
152071-13-1P 152071-14-2P 168466-11-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and catalytic activity of, in olefin **polymerization**)

IT 232-55-3P, 3H-Benz[e]indene 150096-55-2P 150096-60-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation of, with dimethyldichlorosilane, olefin **polymerization** catalysts preparation by)

IT 93903-75-4P 151074-61-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and **decarboxylation** of, olefin **polymn**. catalysts preparation by)

IT 6342-87-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and **dehydration** of, benzoindene derivative from, olefin **polymerization** catalysts preparation by)

IT 150096-53-0P 150096-56-3P 151074-62-3P 151074-63-4P
151074-64-5P 151074-65-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

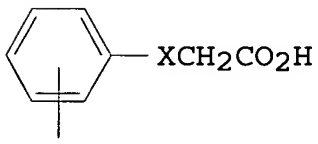
(preparation and reaction of, with zirconium tetrachloride, olefin **polymerization** catalysts preparation by)
IT **21658-35-5P**, 2-Naphthalenepropanoic acid
107777-19-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and sequential chlorination and intramol. Friedel-Crafts
acylation of, benzoindanone derivative from, olefin **polymerization** catalysts preparation by)
IT 150096-54-1P 150096-57-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and sodium borohydride reduction of, benzoindene derivative from,
olefin **polymerization** catalysts preparation by)
IT 20769-85-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acenaphthene, olefin **polymerization** catalysts preparation by)
IT 83-32-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with bromoisobutyryl bromide, olefin **polymn**. catalysts preparation by)

L128 ANSWER 26 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1992:42098 Document No. 116:42098 Following **polymerization** kinetics of multifunctional acrylates in real time by fluorescence probe methodology. Paczkowski, Jerzy; Neckers, D. C. (Cent. Photochem. Sci., Bowling Green State Univ., Bowling Green, OH, 43403, USA). Macromolecules, 25(2), 548-53 (English) 1992. CODEN: MAMOBX. ISSN: 0024-9297.
AB A method is reported which uses dansylamide fluorescence probe methodol. to follow the kinetics of pulsed or continuous laser-initiated **polymerization** and postirradn. processes of trimethylolpropane triacrylate and 1-vinyl-2-pyrrolidinone ,in the presence of acetylated **decarboxylated** Rose Bengal, in real time.
IT **103-01-5**, N-Phenylglycine
RL: USES (Uses)
(trimethylolpropane trimethacrylate photopolymn. in presence of, fluorescence probe for kinetic study in relation to)
RN 103-01-5 HCAPLUS
CN Glycine, N-phenyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

PhNH— CH_2— CO_2H

CC 35-3 (Chemistry of Synthetic High Polymers)
ST kinetics photopolymn fluorescence probe; acrylic **polymn** kinetics photochem
IT Kinetics of **polymerization**
(photochem., of trimethyolopropane trimethacrylate, fluorescence probe methodol. in relation to)
IT 11121-48-5D, Rose Bengal, acetylated, **decarboxylated**
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for photopolymn. of trimethylolpropane trimethacrylate, fluorescence probe methodol. for kinetics in relation to)
IT **103-01-5**, N-Phenylglycine
RL: USES (Uses)
(trimethylolpropane trimethacrylate photopolymn. in presence of, fluorescence probe for kinetic study in relation to)

L128 ANSWER 27 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1991:218092 Document No. 114:218092 Negative-working photosensitive composition. Kawabata, Masami (Nippon Paint Co., Ltd., Japan). Eur. Pat. Appl. EP 386780 A2 19900912, 14 pp. DESIGNATED STATES: R: CH, DE, FR, GB, LI. (English). CODEN: EPXXDW. APPLICATION: EP 1990-104528 19900309. PRIORITY: JP 1989-58188 19890310.
GI



I

AB A neg.-working photosensitive composition which is readily developable in
an aqueous alkaline solution comprises a polymer having a group represented by
the formula N(Ph)CH2CO2H or I (X = O, S, or NR; R = H, CH2CO2H, or C1-3 alkyl). The polymer is **decarboxylated** by
photoreaction of its own or by photoreaction with a photosensitizer

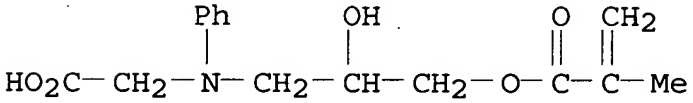
which absorbs light to generate a free radical. The nonexposed areas of the photosensitive composition have carboxylic groups and are dissolved away in the form of salts with an alkaline solution, while the exposed areas lose the carboxylic groups by photodecarboxylation and their solubility in the alkaline solution is greatly reduced by the **polymerization** through free radicals generated at this time. The photosensitive composition is especially useful for forming holograms, printing plates, and resist patterns for printed circuit fabrication.

IT **38807-05-5**
RL: USES (Uses)
(neg.-working photosensitive compns. containing radical-generating photosensitizers and, for forming resist patterns and preparation of printing plates)

RN 38807-05-5 HCAPLUS
CN Glycine, N-[2-hydroxy-3-[(2-methyl-1-oxo-2-propenyl)oxy]propyl]-N-phenyl, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 4896-81-5
CMF C15 H19 N O5



IC ICM G03F007-038
ICS G03F007-039

CC **74-4** (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

IT 9038-42-0 25133-97-5 **38807-05-5** 133601-41-9 133601-43-1
RL: USES (Uses)
(neg.-working photosensitive compns. containing radical-generating photosensitizers and, for forming resist patterns and preparation of printing plates)

L128 ANSWER 28 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1990:402576 Document No. 113:2576 Method of 6-aminopenicillanic acid

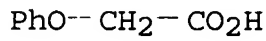
production from phenoxymethylpenicillin with stabilized yeast. Vojtisek, Vladimir; Krumphanzl, Vladimir; Hunkova, Zdenka; Jakubova, Antonia; Bucko, Michal; Miklas, Emil; Culik, Karel (Czech.). Czech. CS 259996 B1 19890511, 18 pp. (Czech). CODEN: CZXXA9. APPLICATION: CS 1987-3060 19870430.

AB Glutaraldehyde-**crosslinked** and (NH4)2SO4-neutralized penicillin V amidase, containing yeast (especially Cryptococcus CCY 17-22-1) are used for manufacture of 6-aminopenicillanic acid (I) from phenoxymethylpenicillin (II). Hydrolysis of II 4-7% weight/volume is carried out at pH 8 and 37°. The immobilized cells may be **dehydrated** with EtOH or Me2CO, dried, and stored for future use. The cells may be used ≥2 times, and phenoxyacetic acid may optionally be recovered from the fermentation medium. The method increases quality and yield of I, decreases time between cycles, and eliminates problems associated with the use of bacteria.

IT **122-59-8P**, Phenoxyacetic acid
RL: PREP (Preparation)
(regeneration of, in aminopenicillanic acid manufacture with immobilized yeast)

RN 122-59-8 HCAPLUS

CN Acetic acid, phenoxy- (8CI, 9CI) (CA INDEX NAME)



IC ICM C12P037-00

CC 7-7 (Enzymes)
Section cross-reference(s): 16

IT Cryptococcus (fungus)
Yeast
(penicillin V amidase-producing, glutaraldehyde **cross-linked**, in aminopenicillanic acid manufacture)

IT 111-30-8, Glutaraldehyde
RL: BIOL (Biological study)
(V-penicillin amidase-producing yeast **cross-linked** with, in aminopenicillanic acid manufacture)

IT **122-59-8P**, Phenoxyacetic acid
RL: PREP (Preparation)
(regeneration of, in aminopenicillanic acid manufacture with immobilized yeast)

L128 ANSWER 29 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1990:180188 Document No. 112:180188 Trialkylsilyloxystyrene polymers

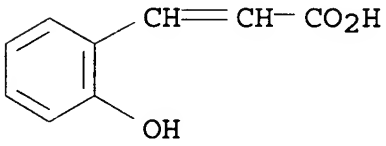
as precursors for poly(2-hydroxystyrene). Yamaguchi, Kazuo; Hirao, Akira; Nakahama, Seiichi (Toa Nenryo Kogyo K. K., Japan). Jpn. Kokai Tokkyo Koho JP 01278504 A2 19891108 Heisei, 4 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1988-107638 19880502.

AB Title polymers have repeating units CH2CH[C6H4(OSiR1R2R3)-o] (I; R1-R3 = C1-6 alkyl) and number-average mol. weight .apprx.500 to .apprx.2000,000. Thus, refluxing 27.78 g coumarin in EtOH in the presence of Na gave 27.50 g o-coumaric acid, 27.02 g of which was **decarboxylated** to give 14.91 g 2-hydroxystyrene, 5.36 g of which was then treated with 6.45 g Me3CSiMe2Cl in DMF in the presence of imidazole to give 6.81 g CH2:CHC6H4(OSiMe2CMe3)-o (II). II was **polymerized** in the presence of 1.07 mol% (based on II) AIBN at 80° for 3 h to give a polymer having repeating units I (R1 = R2 = Me, R3 = CMe3), with number-average mol. weight 21,000, in 58% yield with 71% conversion of II.

IT **583-17-5P**
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and **decarboxylation** of)

RN 583-17-5 HCAPLUS

CN 2-Propenoic acid, 3-(2-hydroxyphenyl)- (9CI) (CA INDEX NAME)



IC ICM C08F012-14

CC 35-8 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): **74**

IT **583-17-5P**
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and **decarboxylation** of)

IT 126590-25-8P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and **polymerization** of)

L128 ANSWER 30 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

1990:180102 Document No. 112:180102 High-molecular-weight poly(2-hydroxystyrene) and its manufacture using a trialkylsilyl protective group. Yamaguchi, Kazuo; Hirao, Akira; Nakahama, Seiichi (Toa Nenryo Kogyo K. K., Japan). Jpn. Kokai Tokkyo Koho JP 01278503 A2 19891108 Heisei, 4 pp. (Japanese). CODEN: JKXXAF. APPLICATION:

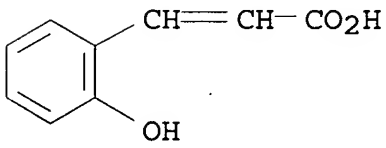
JP 1988-107637 19880502.

AB Poly(2-hydroxystyrene) with number-average mol. weight ≥20,000, useful for photoresists (no data), is manufactured by radical **polymerization** of o-(CH2:CH)C6H4OSiR1R2R3 (I; R1-3 = C1-6 alkyl), followed by hydrolysis of the trialkylsilyl group. Thus, refluxing 27.78 g coumarin in EtOH in the presence of Na gave 27.50 g coumaric acid, 27.02 g of which was **decarboxylated** to give 14.91 g 2-hydroxystyrene, 5.36 g of which was then treated with 6.45 g Me3CSiMe2Cl in DMF to give 6.81 g I (R1 = R2 = Me, R3 = CMe3) (II). II was **polymerized** using 1.07 mol% (based on II) AIBN at 80° for 3 h to give a polymer with number-average mol. weight 21,000 in 58% yield (71% conversion of II). The polymer was treated with Bu4NF in THF to give a product having repeating units CH2CH(C6H4OH-o).

IT **583-17-5P**
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and **decarboxylation** of)

RN 583-17-5 HCAPLUS

CN 2-Propenoic acid, 3-(2-hydroxyphenyl)- (9CI) (CA INDEX NAME)



IC ICM C08F012-14

CC 35-4 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): **74**

ST polyhydroxystyrene manuf high mol wt; alkylsilyloxystyrene radical **polymn** hydrolysis polyhydroxystyrene; photoresist polyhydroxystyrene; silyl protective group polyhydroxystyrene prepn

IT Protective groups
(trialkylsilyl, in preparation of high-mol.-weight poly-o-hydroxystyrene by radical **polymerization**)

IT **583-17-5P**
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and **decarboxylation** of)

IT 126590-25-8P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and radical **polymerization** of)

L128 ANSWER 31 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1990:88342 Document No. 112:88342 Photopolymerizable compositions for negative image formation. Maemoto, Kazuo (Fuji Photo Film Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 01124847 A2 19890517 Heisei, 15 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1987-283490 19871110.

AB The title compns. useful for lithog. plate preparation contain compds. containing ≥1 addition- **polymerizable** ethylenically unsatd. group and carboxy group-containing polymers undergoing photochem. **decarboxylation** in the presence or absence of sensitizers.

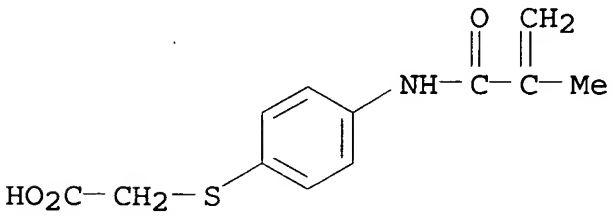
IT **122016-81-3 122016-82-4 125167-61-5**
RL: USES (Uses)
(photosensitive compns. containing, for lithog. plate preparation)

RN 122016-81-3 HCAPLUS

CN 2-Propenoic acid, 2-methyl-, ethyl ester, polymer with [[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]thio]acetic acid (9CI) (CA INDEX NAME)

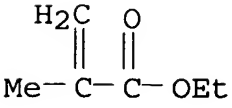
CM 1

CRN 122016-80-2
CMF C12 H13 N O3 S



CM 2

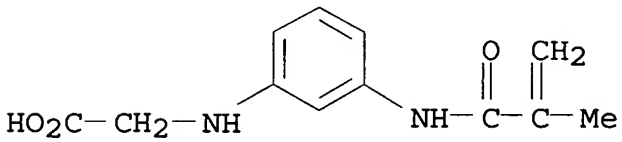
CRN 97-63-2
CMF C6 H10 O2



RN 122016-82-4 HCAPLUS
CN 2-Propenoic acid, 2-methyl-, ethyl ester, polymer with N-[3-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]glycine (9CI) (CA INDEX NAME)

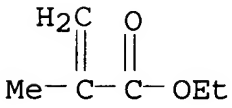
CM 1

CRN 122014-38-4
CMF C12 H14 N2 O3



CM 2

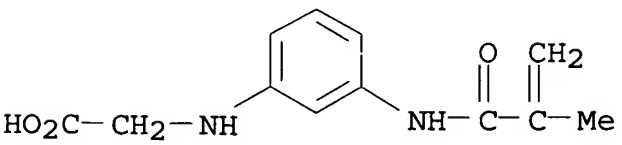
CRN 97-63-2
CMF C6 H10 O2



RN 125167-61-5 HCAPLUS
CN Glycine, N-[3-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]-, polymer with 2-propenyl 2-methyl-2-propenoate (9CI) (CA INDEX NAME)

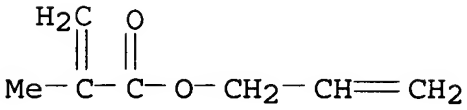
CM 1

CRN 122014-38-4
CMF C12 H14 N2 O3

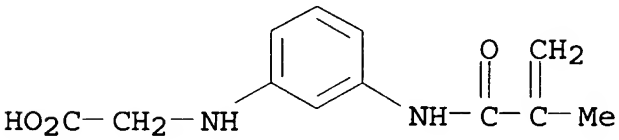


CM 2

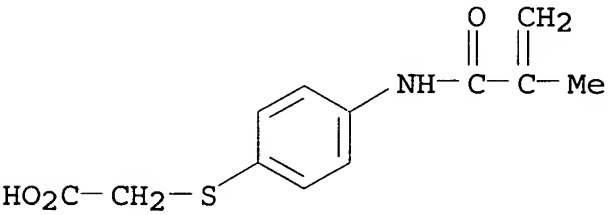
CRN 96-05-9
CMF C7 H10 O2



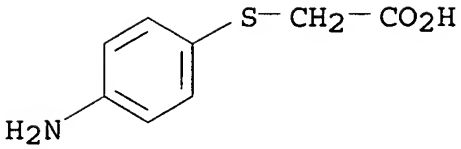
IT **122014-38-4P 122016-80-2P**
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and **polymerization** of)
RN 122014-38-4 HCAPLUS
CN Glycine, N-[3-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]- (9CI) (CA INDEX NAME)



RN 122016-80-2 HCAPLUS
CN Acetic acid, [[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]thio]- (9CI) (CA INDEX NAME)



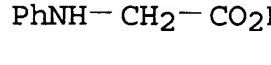
IT **104-18-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of)
RN 104-18-7 HCAPLUS
CN Acetic acid, [(4-aminophenyl)thio]- (9CI) (CA INDEX NAME)



IC ICM G03C001-68
ICS C08F002-44; C08F002-48; C08F002-50; G03C001-68
CC **74-6** (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
ST lithog plate **polymerizable** compn
IT 4755-77-5D, reaction products with polystyrene, hydrolyzed 4986-89-4 9003-53-6D, Polystyrene, reaction products with ethylchlorooxylate, hydrolyzed 15625-89-5, Trimethylolpropane triacrylate 29570-58-9, Dipentaerythritol hexaacrylate **122016-81-3 122016-82-4 125167-61-5**
RL: USES (Uses)
(photosensitive compns. containing, for lithog. plate preparation)
IT **122014-38-4P 122016-80-2P**
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and **polymerization** of)
IT **104-18-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of)

L128 ANSWER 32 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1990:88019 Document No. 112:88019 N-Phenylglycine-(thio)xanthene dye photoinitiating system and application to photopolymer for visible laser exposure. Yamaoka, Tsuguo; Zhang, Yuchuan; Koseki, Kenichi (Fac. Eng., Chiba Univ., Chiba, 260, Japan). Journal of Applied Polymer Science, 38(7), 1271-85 (English) 1989. CODEN: JAPNAB. ISSN: 0021-8995.
AB Bimol. type photoinitiators consisting of N-phenylglycine and (thio)xanthene dyes exhibited high initiating efficiency on irradiation with visible light. A time-resolved spectroscopic study showed that a free radical is formed by the sensitized **decarboxylation** of N-phenylglycine in the presence of (thio)xanthene dye. By using these initiating systems, a visible laser-sensitive photopolymer was prepared, and its imaging characteristics were evaluated.
IT **103-01-5**, N-Phenylglycine

RL: USES (Uses)
(photoinitiator system containing xanthene dye and, for photopolymer
imaging composition)
RN 103-01-5 HCAPLUS
CN Glycine, N-phenyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

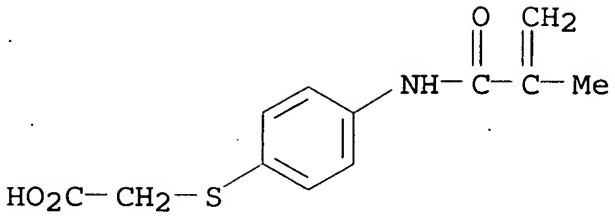


CC **74-4** (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
IT **103-01-5**, N-Phenylglycine
RL: USES (Uses)
(photoinitiator system containing xanthene dye and, for photopolymer
imaging composition)

L128 ANSWER 33 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1989:487423 Document No. 111:87423 Image-producing layer containing carboxyl group-containing polymer. Maemoto, Kazuo (Fuji Photo Film Co., Ltd., Japan). Ger. Offen. DE 3825738 A1 19890302, 13 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1988-3825738 19880728. PRIORITY: JP 1987-188453 19870728.
AB The title material contains a polymer which can be **decarboxylated** by irradiation The material has improved surface stability and adherence to the support. The title material can optionally contain a sensitizer. Thus, Et bromoacetate was reacted with m-aminomethacrylanilide and hydrolyzed to obtain CH2:C(Me)CONH-m-C6H4-NHCH2CO2H (I). I was then copolymd. with Et methacrylate to obtain the imaging material, which was used in the presence of 1-nitronaphthalene as sensitizer.
IT **122016-81-3P 122016-82-4P**
RL: PREP (Preparation)
(preparation and photoimaging composition containing)
RN 122016-81-3 HCAPLUS
CN 2-Propenoic acid, 2-methyl-, ethyl ester, polymer with [[4-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]thio]acetic acid (9CI) (CA INDEX NAME)

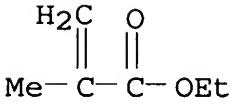
CM 1

CRN 122016-80-2
CMF C12 H13 N O3 S



CM 2

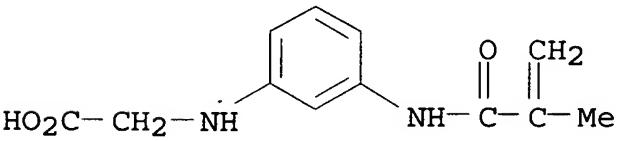
CRN 97-63-2
CMF C6 H10 O2



RN 122016-82-4 HCAPLUS
CN 2-Propenoic acid, 2-methyl-, ethyl ester, polymer with N-[3-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]glycine (9CI) (CA INDEX NAME)

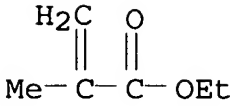
CM 1

CRN 122014-38-4
CMF C12 H14 N2 O3

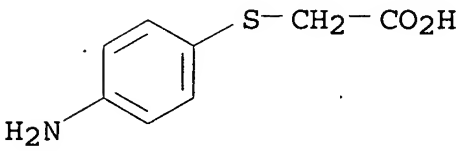


CM 2

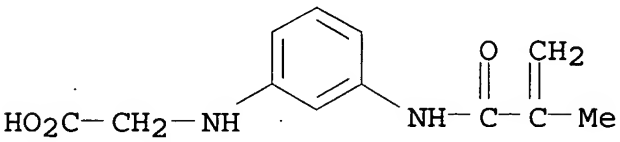
CRN 97-63-2
CMF C6 H10 O2



IT **104-18-7P 122014-38-4P**
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and **polymerization** of, for photoimaging polymer production)
RN 104-18-7 HCAPLUS
CN Acetic acid, [(4-aminophenyl)thio]- (9CI) (CA INDEX NAME)



RN 122014-38-4 HCAPLUS
CN Glycine, N-[3-[(2-methyl-1-oxo-2-propenyl)amino]phenyl]- (9CI) (CA INDEX NAME)



IC ICM G03F007-10
ICS C08L101-02
CC **74-4** (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
IT **122016-81-3P 122016-82-4P**
RL: PREP (Preparation)
(preparation and photoimaging composition containing)
IT **104-18-7P 122014-38-4P**
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and **polymerization** of, for photoimaging polymer production)

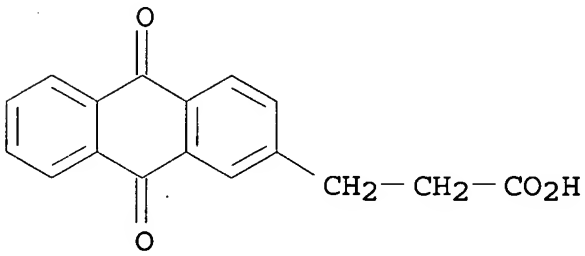
L128 ANSWER 34 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

1989:459600 Document No. 111:59600 Photosensitive compositions containing epoxy resins, alkanolamines, and anthraquinone carboxylic acids. Fischer, Walter; Finter, Juergen (Ciba-Geigy A.-G., Switz.). Eur. Pat. Appl. EP 298033 A2 19890104, 21 pp. DESIGNATED STATES: R: CH, DE, FR, GB, LI, NL. (German). CODEN: EPXXDW. APPLICATION: EP 1988-810429 19880622. PRIORITY: CH 1987-2485 19870701.

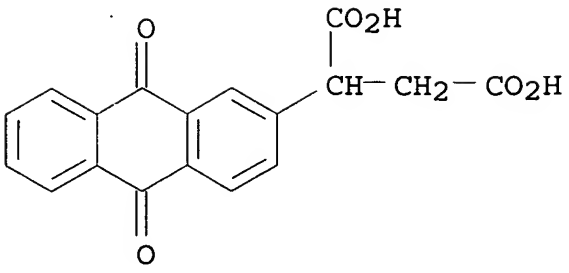
AB Photocurable compns. useful for electroless metalization contain epoxy resins, primary or secondary alkanolamines, and anthraquinones bearing -C(R1)(R2)Z1CO2H groups [R1 = H, alkyl, CN; R2 = H, CN, Z2X (Z2 = direct bond, alkylene; X = CO2H, CN); Z1 = direct bond, alkylene] in the 2-position. A solution of cresol novolak epoxy resin (epoxy equivalent 233.71) 6.04, 2-anthraquinonecarboxylic acid 2.27, and 2-propanolamine 0.676 g in MeOCH2CH2OH containing PhCH2NMe2 was coated on Al and dried at 80° for 12 h to give a film with glass temperature 116° and ratio of efficiency of photoredn. at 385 and 324 nm 0.40.

IT **82203-74-5 121532-50-1 121831-03-6**
RL: MOA (Modifier or additive use); USES (Uses)
(**crosslinking** agents, for epoxy resins by light)

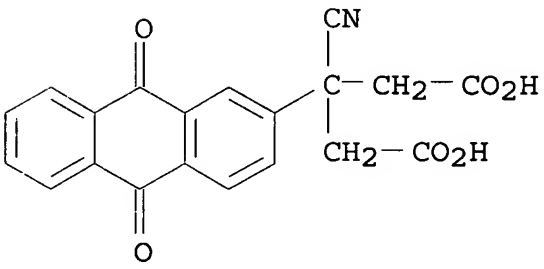
RN 82203-74-5 HCAPLUS
CN 2-Anthracenepropanoic acid, 9,10-dihydro-9,10-dioxo- (9CI) (CA INDEX NAME)



RN 121532-50-1 HCAPLUS
CN Butanedioic acid, (9,10-dihydro-9,10-dioxo-2-anthracenyl)- (9CI) (CA INDEX NAME)



RN 121831-03-6 HCAPLUS
CN Pentanedioic acid, 3-cyano-3-(9,10-dihydro-9,10-dioxo-2-anthracenyl)-
(9CI) (CA INDEX NAME)



IC ICM C08K005-09
ICS C08L063-00; G03C001-00; G03F007-00
CC 42-3 (Coatings, Inks, and Related Products)
Section cross-reference(s): 25, 37, **74**
ST epoxy resin photocurable catalyst; catalyst photochem **crosslinking**; anthraquinonecarboxylic acid catalyst; amino alc catalyst photocuring; propanolamine catalyst photocuring
IT Epoxy resins, uses and miscellaneous
RL: USES (Uses)
(photochem. **crosslinking** agents for, anthraquinonecarboxyl derivs. as)
IT Alcohols, uses and miscellaneous
RL: MOA (Modifier or additive use); USES (Uses)
(amino, **crosslinking** agents, for epoxy resins by light)
IT Phenolic resins, uses and miscellaneous
RL: USES (Uses)
(epoxy, photochem. **crosslinking** agents for, anthraquinonecarboxyl derivs. as)
IT Epoxy resins, uses and miscellaneous

RL: USES (Uses)
(phenolic, photochem. **crosslinking** agents for, anthraquinonecarboxyl derivs. as)

IT **Crosslinking** agents
(photochem., anthraquinonecarboxyl derivs., for epoxy resins)

IT Coating materials
(photocurable, epoxy resins, anthraquinonecarboxyl derivs. as **crosslinking** agents for)

IT 78-96-6D, polymer with dimethyldiglycidylhydantoin and anthraquinonecarboxylic acid 117-78-2D, polymer with dimethyldiglycidylhydantoin and aminopropanol 15336-81-9D, polymer with aminopropanol and anthraquinonecarboxylic acid 121857-05-4 121857-07-6
RL: TEM (Technical or engineered material use); USES (Uses)
(coatings, photochem. **crosslinking** of)

IT 77-86-1 78-96-6, 1-Amino-2-propanol 117-78-2, 2-Anthraquinonecarboxylic acid 141-43-5, Ethanolamine, uses and miscellaneous 4048-33-3 13325-10-5, 4-Amino-1-butanol 76161-80-3 **82203-74-5 121532-50-1 121831-03-6** 121831-06-9 121831-08-1
RL: MOA (Modifier or additive use); USES (Uses)
(**crosslinking** agents, for epoxy resins by light)

IT 9016-83-5D, Cresol-formaldehyde copolymer, glycidyl ethers
RL: USES (Uses)
(photochem. **crosslinking** agents for, anthraquinonecarboxyl derivs. as)

IT 121532-49-8P 121831-00-3P 121831-02-5P
RL: PREP (Preparation)
(preparation, saponification and **decarboxylation** of)

L128 ANSWER 35 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1989:458841 Document No. 111:58841 Investigations on the **curing** of epoxy resins with hexahydrophthalic anhydride. Steinmann, Bettina (Ciba-Geigy Ltd., Fribourg, CH-1701, Switz.). Journal of Applied Polymer Science, 37(7), 1753-76 (English) 1989. CODEN: JAPNAB. ISSN: 0021-8995.

AB Polymers of bisphenol A diglycidyl ether and diglycidyl hexahydrophthalate as well as Ph glycidyl ether and cyclohexanecarboxylic acid glycidyl ester were **cured** with hexahydrophthalic anhydride (I) in the presence of benzyldimethylamine or 1-methylimidazole as catalysts at 100-140°. Investigations of the **curing** kinetics gave sigmoidal-shaped curves with marked induction periods. **IR** anal. of the **cured** products revealed that the propagation proceeds not only by the esterification reaction of

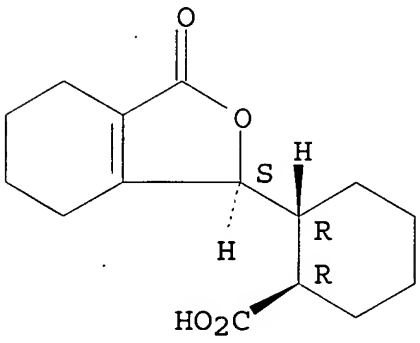
epoxide with anhydride but also by chain anhydride formation by the reaction of carboxylate with anhydride groups. 13C-NMR investigations of the soluble polymers showed that most of the peaks resulting from double bonds could not be assigned to structures formed by initiation reactions that had previously been proposed for the anhydride **curing** of epoxides. In analogy to a postulated mechanism for the **decarboxylation** condensation of I alone in the presence of tertiary amines, it is proposed that an isomerization product of I is one of the mols. that initiate the **curing** reaction.

IT **100419-22-5P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from isomerization-**decarboxylation** of hexahydrophthalic anhydride as **crosslinking** agent for epoxy resins, **curing** mechanism in relation to)

RN 100419-22-5 HCAPLUS

CN Cyclohexanecarboxylic acid, 2-(1,3,4,5,6,7-hexahydro-3-oxo-1-isobenzofuranyl)-, [1α,2β(S*)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



CC 37-6 (Plastics Manufacture and Processing)
Section cross-reference(s): 35

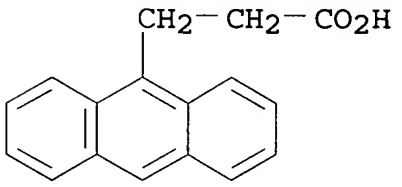
ST **crosslinking** epoxy resin hexahydrophthalic anhydride; bisphenol diglycidyl ether **crosslinking** anhydride; phenyl glycidyl ether **crosslinking** anhydride; cyclohexanecarboxylic acid glycidyl ester **crosslinking**; mechanism **crosslinking** epoxy hexahydrophthalic anhydride; kinetics **crosslinking** epoxy hexahydrophthalic anhydride

IT **Crosslinking** catalysts
(benzyldimethylamine and methylimidazole, for epoxy resins with hexahydrophthalic anhydride, mechanism and kinetics in relation to)

IT Epoxy resins, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(**crosslinking** of, with hexahydrophthalic anhydride, mechanism and kinetics of)
IT **Crosslinking** agents
(hexahydrophthalic anhydride, for epoxy resins, mechanism and kinetics in relation to)
IT Kinetics of **crosslinking**
(of epoxy resins, with hexahydrophthalic anhydride)
IT **Crosslinking**
(of epoxy resins, with hexahydrophthalic anhydride, mechanism of)
IT 103-83-3, Benzyldimethylamine 616-47-7, 1-Methylimidazole
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for **crosslinking** of epoxy resins with hexahydrophthalic anhydride, mechanism and kinetics in relation to)
IT 25085-99-8 27103-66-8 121594-99-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(**crosslinking** of, with hexahydrophthalic anhydride, mechanism and kinetics of)
IT 85-42-7, Hexahydrophthalic anhydride
RL: USES (Uses)
(**crosslinking** with, of epoxy resins, mechanism and kinetics of)
IT **100419-22-5P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from isomerization-**decarboxylation** of hexahydrophthalic anhydride as **crosslinking** agent for epoxy resins, **curing** mechanism in relation to)

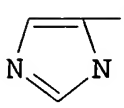
L128 ANSWER 36 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1987:176960 Document No. 106:176960 Cationic ring opening **polymerization** of 4,5-dihydro-2-[2-(9-anthryl)ethyl]-1,3-oxazole. Simionescu, Christofor I.; Onofrei, Geta; Grigoras, Mircea ("P. Poni" Inst. Macromol. Chem., Iasi, 6600, Rom.). Makromolekulare Chemie, 188(3), 505-11 (English) 1987. CODEN: MACEAK. ISSN: 0025-116X.
AB 4,5-Dihydro-2-[2-(9-anthryl)ethyl]-1,3-oxazole [107674-13-5] was synthesized and **polymerized** by cationic ring-opening isomerization. The **polymerization** was carried out in bulk or in solution, using Me tosylate [80-48-8], ethylene ditosylate [6315-52-2] and α-tosyl-ω-tosyloxypoly(oxyethylene) [35164-96-6] as initiators. The polymers were characterized by **IR**, 1H NMR and UV spectroscopy.
IT **41034-83-7P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with ethanolamine)
RN 41034-83-7 HCAPLUS
CN 9-Anthracenepropanoic acid (9CI) (CA INDEX NAME)



CC 35-7 (Chemistry of Synthetic High Polymers)
ST dihydroanthrylethyloxazole polymer; polydihydroanthrylethyloxazole; tosylate **polymn** catalyst dihydroanthrylethyloxazole
IT **Polymerization** catalysts
(ring-opening, tosylates, for dihydro(anthrylethyl)oxazole)
IT 80-48-8, Methyl tosylate 6315-52-2 35164-96-6
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for ring-opening **polymerization** of dihydro(anthrylethyl)oxazole)
IT 61161-88-4, Diethyl (9-anthryl)methylmalonate
RL: RCT (Reactant); RACT (Reactant or reagent)
(**decarboxylation** of)
IT 107674-13-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and **polymerization** of)
IT **41034-83-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with ethanolamine)

L128 ANSWER 37 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1986:470178 Document No. 105:70178 Base precursors for heat-developable photosensitive materials. Sato, Kozo; Yabuki, Yoshiharu; Hirai, Hiroyuki; Kawata, Ken (Fuji Photo Film Co., Ltd. , Japan). Ger. Offen. DE 3530063 A1 19860306, 83 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1985-3530063 19850822. PRIORITY: JP 1984-176400 19840824.
GI



I

AB Heat-developable, photosensitive materials having an outstanding stability and capable of producing a high d. image with low fog in a short time span contain a base precursor of the RR1C:CR2CO2H.B (R = a **decarboxylation** accelerating group; R1, R2 = H, alkyl, cycloalkyl, alkenyl, alkynyl, aralkyl, aryl, hetercyclyl, CO2H or a salt thereof, halo, CN, alkylsulfonyl, arylsulfonyl, sulfamoyl, carbamoyl, alkoxycarbonyl, aryloxycarbonyl, di- or monoalkylphosphoryl, di- or monoarylphosphenyl, alkylsulfinyl, arylsulfinyl, acyl, NH2, acylamino, or acyloxy; B = an organic base; n = 1 or 2). Thus, a PET film support was coated at 30 μm (wet) with a composition containing a **gelatin**-Ag(Br,I) emulsion 25, a dispersion of a dye-releasing compound 33, I 3.1 g, a 10% aqueous solution of Me2NSO2NH2 4, and water 20 mL, dried, imagewise exposed for 10 s to a 2000 lx W lamp, heated for 20 s at 150°, combined with an image receptor, and heated for 6 min at 80° to give a neg. magenta image with a dmax of 1.99 and a Dmin of 0.21 vs. 1.28 and 0.16, resp., for a I-free control.

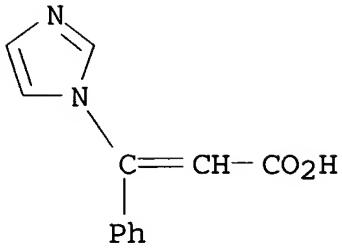
IT **103406-08-2 103406-10-6 103406-12-8**
103406-14-0 103426-14-8
RL: USES (Uses)
(color photothermog. copying material containing, as base precursor)

RN 103406-08-2 HCAPLUS

CN 2-Propenoic acid, 3-(1H-imidazol-1-yl)-3-phenyl-, compd. with guanidine (1:1) (9CI) (CA INDEX NAME)

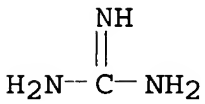
CM 1

CRN 103406-07-1
CMF C12 H10 N2 O2



CM 2

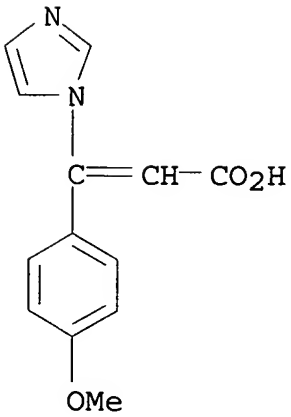
CRN 113-00-8
CMF C H5 N3



RN 103406-10-6 HCAPLUS
CN 2-Propenoic acid, 3-(1H-imidazol-1-yl)-3-(4-methoxyphenyl)-, compd. with guanidine (1:1) (9CI) (CA INDEX NAME)

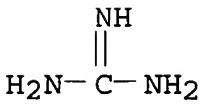
CM 1

CRN 103406-09-3
CMF C13 H12 N2 O3



CM 2

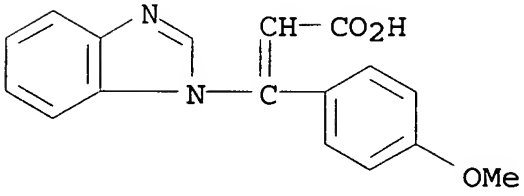
CRN 113-00-8
CMF C H5 N3



RN 103406-12-8 HCAPLUS
CN 2-Propenoic acid, 3-(1H-benzimidazol-1-yl)-3-(4-methoxyphenyl)-, compd. with guanidine (1:1) (9CI) (CA INDEX NAME)

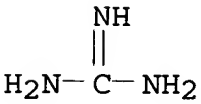
CM 1

CRN 103406-11-7
CMF C17 H14 N2 O3



CM 2

CRN 113-00-8
CMF C H5 N3

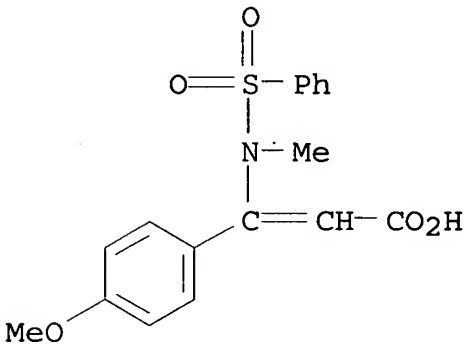


RN 103406-14-0 HCAPLUS
CN 2-Propenoic acid, 3-(4-methoxyphenyl)-3-

[methyl(phenylsulfonyl)amino]-, compd. with guanidine (1:1) (9CI) (CA INDEX NAME)

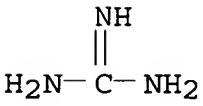
CM 1

CRN 103406-13-9
CMF C17 H17 N O5 S



CM 2

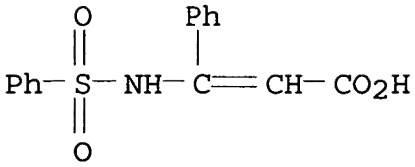
CRN 113-00-8
CMF C H5 N3



RN 103426-14-8 HCAPLUS
CN 2-Propenoic acid, 3-phenyl-3-[(phenylsulfonyl)amino]-, compd. with guanidine (1:1) (9CI) (CA INDEX NAME)

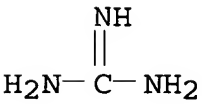
CM 1

CRN 103426-13-7
CMF C15 H13 N O4 S



CM 2

CRN 113-00-8
CMF C H5 N3



IC ICM G03C001-42
CC **74-7** (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
IT **103406-08-2 103406-10-6 103406-12-8 103406-14-0 103426-14-8**
RL: USES (Uses)
(color photothermog. copying material containing, as base precursor)

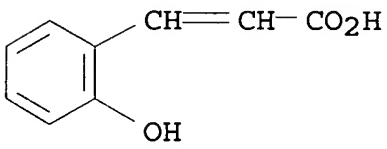
L128 ANSWER 38 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1984:414928 Document No. 101:14928 Color development and insolubilization by the reaction of nitrene with poly(o-hydroxystyrene). Koseki, Kenichi; Yamaoka, Tsuguo (Fac. Eng., Chiba Univ., Chiba, 260, Japan). Nippon Kagaku Kaishi (12), 1708-14 (Japanese) 1983. CODEN: NKAKB8. ISSN: 0369-4577.
AB Poly(o-hydroxystyrene) (I) was obtained by radical **polymerization** of o-hydroxystyrene monomer which was synthesized by **decarboxylation** of o-coumaric acid. A film prepared from I and aromatic azide compds. resulted in photosensitivity for UV and visible light. The film was colored and insolubilized in alkaline solns. by irradiation with active light. The color change was versatile according to the mol. structure of the aromatic azide compds. used. A film of I with p-dimethylaminophenyl azide gave a deep blue color image by imagewise exposure. The mechanisms of the photocoloration

and photocuring of I films by aromatic azide compds. were investigated by using o-cresol as a monomeric model compound for I. The photoinduced color development was attributable to the formation of a dye having a quinone-imine structure through the reaction of nitrene, formed by the photolysis of aromatic azide compds., with the phenol group of I. The decrease in the solubility of the exposed I/azide
film in alkaline solns. could be explained by the change in solubility parameter of I owing to the reduced OH group by the formation of the quinone-imine structure.

IT **583-17-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**decarboxylation** of, in preparation of hydroxystyrene in preparation of photoresists and photoimaging materials)

RN 583-17-5 HCAPLUS

CN 2-Propenoic acid, 3-(2-hydroxyphenyl)- (9CI) (CA INDEX NAME)



CC **74-5** (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

IT **583-17-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**decarboxylation** of, in preparation of hydroxystyrene in preparation of photoresists and photoimaging materials)

L128 ANSWER 39 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

1984:157023 Document No. 100:157023 Studies on the **polymerization** of functional monomers containing amino groups. V. Synthesis of 4-N,N-dimethylaminostyrene and its use as a component of the redox initiation system. Li, Fumian; Cui, Qiang; Feng, Xinde (Dep. Chem., Peking Univ., Beijing, Peop. Rep. China). Gaofenzi Tongxun (5), 396-400 (Chinese) 1983. CODEN: KFTTAR. ISSN: 0453-2880.

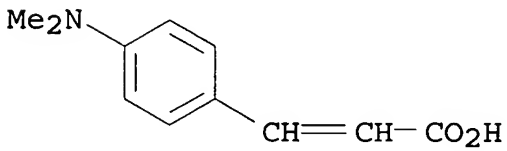
AB 4-N,N-Dimethylaminostyrene (I) [2039-80-7] hardly underwent **radical polymerization initiated** by organic peroxides such as benzoyl peroxide (II) [94-36-0] and lauroyl peroxide, but it formed a redox system at low concentration with II to initiate the **polymerization** of Me methacrylate (III). The rate equation of the **polymerization** of I was Rp =

Kp[III][I]0.5[II]0.5, and the activation energy of **polymerization** was 7.4 kcal/mol. I initiated the **polymerization** and also entered into the polymer chains.

IT **1552-96-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**decarboxylation** of, to dimethylaminostyrene)

RN 1552-96-1 HCAPLUS

CN 2-Propenoic acid, 3-[4-(dimethylamino)phenyl]- (9CI) (CA INDEX NAME)



CC 35-3 (Chemistry of Synthetic High Polymers)

IT **Decarboxylation**
(of dimethylaminocinnamic acid, to dimethylaminostyrene)

IT **Polymerization** catalysts
(redox, dimethylaminostyrene and benzoyl peroxide, for Me methacrylate)

IT Kinetics of **polymerization**
(redox, of Me methacrylate)

IT 2039-80-7
RL: CAT (Catalyst use); USES (Uses)
(catalysts, containing benzoyl peroxide, for **polymerization** of Me methacrylate)

IT 94-36-0, uses and miscellaneous
RL: CAT (Catalyst use); USES (Uses)
(catalysts, containing dimethylaminostyrene, for **polymerization** of Me methacrylate)

IT **1552-96-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**decarboxylation** of, to dimethylaminostyrene)

L128 ANSWER 40 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

1983:496689 Document No. 99:96689 The zinc tetraphenylporphin-sensitized photoredox reaction between N-phenylglycine and p-benzoquinone in polar solvents. Nishimoto, Seiichi; Tada, Hiroaki; Kagiya, Tsutomu (Dep. Hydrocarbon Chem., Kyoto Univ., Kyoto, 606, Japan). Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (6), 873-7

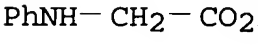
(English) 1983. CODEN: JCPKBH. ISSN: 0300-9580.

AB The photoredox reaction between N-phenylglycine (I) and p-benzoquinone (II) sensitized by Zn tetraphenylporphine (III) was studied in various solvents under N at 25°. **Decarboxylation** of I and reduction of II occurred equimol. to give PhN:CH2, CO2, and 1,4-(HO)2C6H4 when a MeCN solution of I and II was irradiated at >500 nm in the presence of a catalytic amount of III. III was recovered almost quant. after the photoreaction. The conversion of I increased linearly with increasing the molar ratio of III to I up to .apprx.2 + 10-3. The quantum yield for the III-sensitized **decarboxylation** of I in N-purged MeCN solution was 0.20. The sensitizing activity of III was remarkably enhanced upon increasing the solvent polarity.

IT **103-01-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**decarboxylation** of, in photoredox reaction with benzoquinone in presence of zinc tetraphenylporphine)

RN 103-01-5 HCAPLUS

CN Glycine, N-phenyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC **74-1** (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 22

ST phenylglycine benzoquinone photoredox; zinc phenylporphine sensitizer photoredox; **decarboxylation** phenylglycine redn benzoquinone

IT **Decarboxylation**
(of phenylglycine, in photoredox reaction with benzoquinone in presence of zinc tetraphenylporphine)

IT **103-01-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**decarboxylation** of, in photoredox reaction with benzoquinone in presence of zinc tetraphenylporphine)

L128 ANSWER 41 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

1978:611116 Document No. 89:211116 Synthesis of dehydropolymers using a system simulating tyrosinase properties. Gravitis, J.; Stoldere, I. (Inst. Khim. Drev., Riga, USSR). Koksnes Kimija (5), 68-73 (Russian) 1978. CODEN: KHDRDQ. ISSN: 0201-7474.

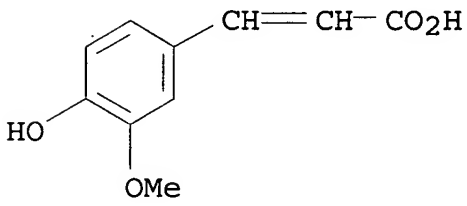
AB Using CuCl-pyridine complex as a model tyrosinase system, dehydropolymers were formed from the substrate, ferulic acid. Anal.

of the products by **gel** chromatog., UV and **IR** spectroscopy, differential thermal anal., and high-frequency titration showed that the dehydropolymers had a **crosslinked** structure and a multimodal mol. weight distribution. In the synthesis reaction, **decarboxylation** processes also occurred in addition to dehydration.

IT **1135-24-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydropolymn. of, by tyrosinase model system)

RN 1135-24-6 HCAPLUS

CN 2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)- (9CI) (CA INDEX NAME)



CC 7-4 (Enzymes)

IT **1135-24-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydropolymn. of, by tyrosinase model system)

L128 ANSWER 42 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

1977:190632 Document No. 86:190632 Thermal degradation of polymers. XV. Vacuum pyrolysis studies on poly(p-methoxystyrene) and poly(p-hydroxystyrene). Still, R. H.; Whitehead, A. (Dep. Polym. Fibre Sci., Univ. Manchester Inst. Sci. Technol., Manchester, UK). Journal of Applied Polymer Science, 21(5), 1199-213 (English) 1977. CODEN: JAPNAB. ISSN: 0021-8995.

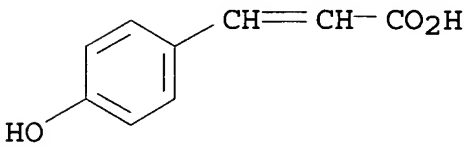
AB Poly(p-hydroxystyrene) (I) [24979-70-2] showed anomalous behavior during vacuum pyrolysis at 300-500° resulting from the high reactivity of p-hydroxystyrene (II) [2628-17-3] monomer and the facility for transfer afforded by the proton of the hydroxyl substituent. The products of degradation were identified and quant. and qual. analyzed and the degradation behavior of the two systems compared with polystyrene. A mechanism is proposed for the degradation of I and of poly(p-methoxystyrene) [24936-44-5]. In addition the preparation and

free radical **polymerization** of II and p-methoxystyrene [637-69-4] is described. The **polymerization** behavior of II is anomalous, and a mechanism is suggested to account for the phenomenon.

IT **7400-08-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and **decarboxylation** of)

RN 7400-08-0 HCAPLUS

CN 2-Propenoic acid, 3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



CC 35-6 (Synthetic High Polymers)

ST polymethoxystyrene thermal degrdn mechanism; polyhydroxystryene thermal degrdn mechanism; **polymn** mechanism hydroxystyrene; substituent effect polystyrene degrdn

IT **Polymerization**
(radical, of substituted styrenes, mechanism of)

IT **7400-08-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and **decarboxylation** of)

IT 3319-15-1P
RL: PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation and **dehydration** of)

IT 637-69-4P 2628-17-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and **polymerization** of, mechanism of)

L128 ANSWER 43 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

1973:453807 Document No. 79:53807 Stable oxygen polyradicals. I. Synthesis of **polymerizable** monomers possessing a sterically hindered free of protected phenolic hydroxyl group. Braun, Dietrich; Maier, Bertold (Dtsch. Kunstst. Inst., Darmstadt, Fed. Rep. Ger.). Makromolekulare Chemie, 167, 119-77 (German) 1973. CODEN: MACEAK. ISSN: 0025-116X.

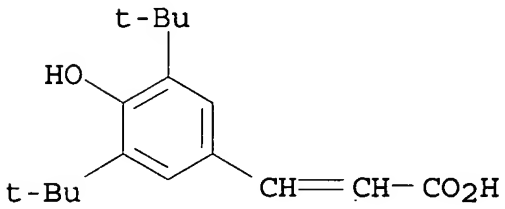
AB 2,6-Tert-butyl-4-vinylphenol [19263-36-6] was prepared by **decarboxylating** the corresponding 3-arylacrylic acid.

2,6-Di-tert-butyl-4-isopropenylphenol [19263-37-7] was prepared by **dehydrating** the corresponding 2-aryl-2-propanol. 2,6-Di-tert-butyl-4-isopropenylphenyl methyl ether (I) [41476-08-8] was similarly prepared

IT **22014-01-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**decarboxylation** of)

RN 22014-01-3 HCAPLUS

CN 2-Propenoic acid, 3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]- (9CI) (CA INDEX NAME)



CC 35-2 (Synthetic High Polymers)
Section cross-reference(s): 25

IT **22014-01-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**decarboxylation** of)

IT 1344-28-1, uses and miscellaneous
RL: USES (Uses)
(**dehydration** of [bis(tert-butyl)hydroxyphenyl]propanol in presence of)

IT 7664-38-2, uses and miscellaneous
RL: USES (Uses)
(**dehydration** of [bis(tert-butyl)methoxyphenyl]propanol in presence of)

IT 24830-01-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(**dehydration** of, with aluminum oxide)

IT 42567-42-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(**dehydration** of, with phosphoric acid)

L128 ANSWER 44 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1965:43837 Document No. 62:43837 Original Reference No. 62:7732c-e
Catalytic hydrogenation of pyridinecarboxylic acids and pyridylalkanecarboxylic acids. Freifelder, Morris (Abbott Laboratories). US 3159639 19641201, 2 pp. (Unavailable).

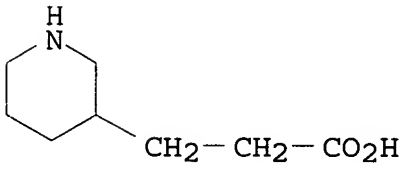
APPLICATION: US 19620917.

AB Hydrogenation takes place in the presence of a Rh catalyst and an equimolar amount of NH3. Good yields are obtained at room temperature and between 1 and 3 atmospheric H pressure. Nicotinic acid (6.15 g.) in 50 cc. H2O and 5.5 cc. concentrated aqueous NH3 in a Parr shaker was treated with 2.4 g. 5% Rh-Al2O3 and the mixture hydrogenated at 2 atmospheric to give 88.5% nipecotic acid, m. 260-1°. Similarly prepared were: pipecolic acid, m. 276°; isonipecotic acid, m. 336°; 3-piperidinepropionic acid, 94%, m. 180-1°; 4-piperidinepropionic acid, 89%, m. 275-7°. An aqueous solution of 2.5 g. pyridineacetic acid-HCl was passed through a column of Amberlite **IR**-120 and eluted with 2.5% aqueous NH3. The eluate was evaporated and the residue dissolved in H2O and hydrogenated as described to give 64.5% 4-piperidineacetic acid.

IT **1822-31-7**, 3-Piperidinepropionic acid **1822-32-8**, 4-Piperidinepropionic acid
(preparation of)

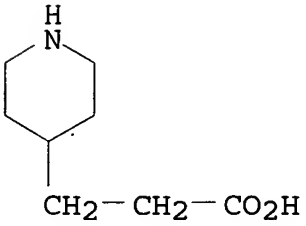
RN 1822-31-7 HCAPLUS

CN 3-Piperidinepropanoic acid (9CI) (CA INDEX NAME)



RN 1822-32-8 HCAPLUS

CN 4-Piperidinepropanoic acid (9CI) (CA INDEX NAME)



INCL 260293200
CC 37 (Heterocyclic Compounds (One Hetero Atom))
IT Acids
(catalysts in **polymerization**, pyridylalkyl, hydrogenation of)
IT 32075-31-3, Pyridinecarboxylic acid
(**decarboxylation** of, hydrogenation of)
IT **1822-31-7**, 3-Piperidinepropionic acid **1822-32-8**, 4-Piperidinepropionic acid
(preparation of)

L128 ANSWER 45 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1965:29905 Document No. 62:29905 Original Reference No. 62:5331d-h,5332a-h Thermal **decarboxylation** of α-amino acids. Chatelus, Georges (Ecole Natl. Super. Chim., Clermont-Ferrand). Bulletin de la Societe Chimique de France (10), 2523-32 (French) 1964. CODEN: BSCFAS. ISSN: 0037-8968. OTHER SOURCES: CASREACT 62:29905.

AB The thermal **decarboxylation** of α-amino acids in an inert medium was noticeably accelerated by organic peroxides and led always to the amine having the same structure as the starting amino acid. The **decarboxylation** proceeded with more or less speed in the presence of ketones (or aldehydes) with the intermediate formation of the Schiff base to yield, in most cases, the amine with the same C-skeleton as the starting acid. Only certain acids with a quaternary α-C atom undergo a complete transamination. The course of the reaction is a function of the nature of the amino acids and not of the ketone employed. A series of runs was performed to determine the effect of various reaction conditions and media on the **decarboxylation** of DL-leucine in the absence or presence of catalysts, such as tetralin peroxide (II), azo(bisisobutyronitrile) (III), and FeSO4; the conditions and results of these runs are given in the 1st table. The crude **decarboxylation** product from DL-leucine in BzMe distilled gave iso-AmNH2, b730 90-1°,BzMe, b12 85-90°, and a viscous mixture, b12 120° to b2 190°, containing 3-40% iso-AmN:CMePh. reaction medium, catalyst, temperature, time in hrs., %
yield iso-AmNH2; distilled Tetralin, 2% II, 170°, 6, 80; pure Tetralin, 0.2% II, 160°, 5, 10; purified Tetralin, 1% II, 170°, 6, 95; distilled Tetralin, 1% FeSO4, 160°, 7, 28; Decalin, --, 180°, 5, 3; Decalin, 1% II, 180°, 5, 40; saturated hydrocarbon, 1% II, 185°, 7, 50; saturated hydrocarbon, 2% III, 150°, 8, 10; squalane, --, 190°, 8, 22; squalane, 1% II, 190°, 8, 45; dodecene, --, 190°, 5, 20;

dodecene, 0.5% II, 190°, 5, 40; alkylbenzene, --, 190°, 4, 35; alkylbenzene, 1% II, 190°, 4, 85; 1-C10H7Me, 1% II, 180°, 5, 90; poly(ethylene glycol) 300, --, 180°, 8, 80; dodecylpoly(ethylene glycol), --, 180°, 8, 84; Carbitol, --, 180°, 6, 65; (CH2OH)2, --, 160°, 4, 6; veratrole, --, 180°, 3, 4; veratrole, II, 180°, 3, 90; C6H3Cl3, --, 190°, 8, 55; 1-C10H7Cl, II, 180°, 8, 85; PhNO2, II, 190°, 8, 50; Me2SO, --, 180°, 5, 82; HCONHMe, II, 170°, 7, 85; quinoline, --, 160°, 3, 75; BzOEt-o-C6H4(CO2Et)2, II, 160°, 6, 85; BzMe and sec-BuNH2 heated with a trace of PhNH2-ZnCl2 under pressure at 140° yielded sec- BuN:CMePh, b12 110-12°. A series of **decarboxylation** runs was performed with DL-leucine in inert media in the presence of ketones; the conditions and results of the runs are listed in the 2nd table. The **decarboxylation** in the presence of ketones (oraldehydes) was studied with the compds. listed in the 3rd table. reaction medium, ketone used, mole ratio amino acid-ketone, temperature, time hrs., % yield iso-AmNH2; Tetralin, tetralone, 1.5, 160°, 7, 95; Tetralin, cyclohexanone (IV), 1.5, 165°, 6, 94; squalane, IV, 1.5, 180°, 8, 60; squalane, tetralone, 1.5, 180°, 8, 75; squalane, BzMe, 1, 175°, 5, 84; poly(ethylene glycol), tetralone, 2, 165°, 6, 80; amino acid used, carbonyl used, molar ratio acid-ketone, temperature, time in hrs., product, % yield; leucine, Am2CO, 0.32, 150°, --, iso-AmNH2, 71; leucine, iso-Bu2CO, 0.28, 150-130°, -, iso-AmNH2, 44; leucine, cyclopentanone, 0.20, 130°, --, iso-AmNH2, 29; leucine, IV, 0.10, 150-130°, --, iso-AmNH2, 50; leucine, cycloheptanone, 0.20, 130°, --, iso-AmNH2, 97; leucine, methylcyclohexanones (V), 0.13, 160-145°, --, iso-AmNH2, 98; leucine, camphor, 0.38, 180-130°, --, iso-AmNH2, 85; leucine, Ph2CO, 0.40, 170-130°, 6, iso-AmNH2, 90; leucine, p-MeOC6H4CHO, 0.27, 130°, --, iso-AmNH2, 100; leucine, BzMe, 0.20, 150°, 4, iso-AmNH2, 99; leucine, AcCH2Ph (VI), 0.26, 150-120°, --, iso-AmNH2, >80; valine, BzMe, 0.26, 140-125°, 6, iso-BuNH2, 85; Me2C(NH2)CO2H, BzMe, 0.25, 155°, 6, MePbCHNH2 (VII), 27; isovaline (VIII), BzMe, 0.26, 155°, 4, --, 40-50; VIII, BzEt, 0.27, 150-130, --, VII, 30; VIII, Ph2CO, 0.21, 180-140°, 6, Ph2CHNH2, 35; VIII, nonanone (IX), 0.20, 165°, --, C9H19NH2, 4; VIII, IV, 0.28, 155°, --, VII, <20; VIII, p-MeC6H4Ac (X), 0.24, 130°, --, p-MeC6H4CH(NH2)Me, 32; VIII, p-MeOC6H4CHO, 0.23, 120°, 3.5, p-MeOC5H4NH2, 100; norvaline, BzMe, 0.21, 165°, 5, BuNH2, 80; threonine, BzMe, 0.15, 130°, 4,

MeCH(OH)CH2NH2, 99; lysine, BzMe, 0.11, 140°, 6, cadaverine, 6; methionine, BzMe, 0.20, 120°, 3.5, MeS(CH2)3NH2, 100; iso-BuCH(Co2H)NHMe, BzMe, 0.18, 155°, 2, iso-AmNHMe, 92; PhNHCH2CO2H, BzMe, 0.15, 150°, 3, MeNHPh, 98; PhCH2CH(NH2)CO2H, BzMe, 0.20, 130°, 3, PhCH2CH2NH2, 100; PhCH(NH2)CO2H, BzMe, 0.15, 135°, 4, PhCH2NH2, 100; MePhC(NH2)CO2H (XI), BzMe, 0.13, 140°, 4, VII, 81; XI, BzEt, 0.16, 150°, --, VII + EtPhCHNH2, 91; XI, VI, 0.17, 125°, --, VII + MePhCHCH(NH2)CH2NH2, ≥93; XI, IX, 0.17, 165°, 14, VII + iso-Pr2CHNH2, 72; XI, IV, 0.10, 110°, --, VII + cyclohexylamine, 100; XI, X, 0.15, 150°, --, VII + p-MeC6H4CH2CH2NH2, 96; Ph2C(NH2)CO2H, BzMe, 0.15, 130°, 5, Ph2NME, 90; tyrosine, BzMe, 0.17, 145°, 5, p-HOC6H4CH2CH2NH2, 80; tryptophan, BzMe, 0.15, 130°, 4 , tryptamine, 100; proline, BzMe, 0.20, 120°, 4, pyrrolidine, 70; 1-aminocyclopentanecarboxylic acid, BzMe, 0.14, 145°, 4, VII, 60; 1-aminocyclohexanecarboxylic acid (XII), BzMe, 0.15, 160°, 4, VII, 60; XII, IX or IV, 0.18, 160°, --, VII, about 5; XII, V, 0.16, 155°, --, VII, about 5; iso-BuCH(CO2H)NME2, BzMe, 0.13, 200°, 4, --, 0;

IT **103-01-5**, Glycine, N-phenyl-
(carboxyl group removal from)

RN 103-01-5 HCAPLUS

CN Glycine, N-phenyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

PhNH—CH_2—CO_2H

CC 44 (Amino Acids, Peptides, and Proteins)

IT Acids
(catalysts in **polymerization**, reactions of, with aliphatic amines)

IT Solvents
(in amino acid **decarboxylation**)

IT 52-52-8, Cyclopentanecarboxylic acid, 1-amino- 56-87-1, Lysine 60-18-4, Tyrosine 61-90-5, Leucine 62-57-7, Alanine, 2-methyl- 63-68-3, Methionine 72-18-4, Valine 72-19-5, Threonine **103-01-5**, Glycine, N-phenyl- 147-85-3, Proline 565-07-1, Alanine, 2-phenyl- 595-40-4, Isovaline 2439-37-4, Leucine, N,N-dimethyl- 2756-85-6, Cyclohexanecarboxylic acid, 1-amino- 2835-06-5, Glycine, 2-phenyl- 3060-46-6, Leucine, -methyl- 3060-50-2, Glycine, 2,2-diphenyl- 6600-40-4, Norvaline
(carboxyl group removal from)

IT 63-91-2, Alanine, phenyl-

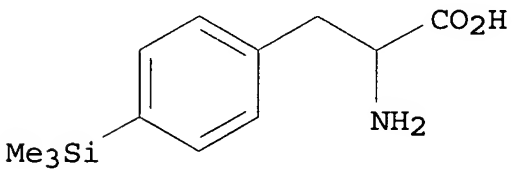
(**decarboxylation** of)

L128 ANSWER 46 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1964:3549 Document No. 60:3549 Original Reference No. 60:651g
Synthesis of DL-p-trimethylsilylphenylalanine. Frankel, Max; Gertner, David; Shenhar, Avinoam; Zilkha, Albert (Hebrew Univ., Jerusalem). Journal of the Chemical Society, Abstracts (Nov.), 5049-51. (Unavailable) 1963. CODEN: JCSAAZ. ISSN: 0590-9791. OTHER SOURCES: CASREACT 60:3549.

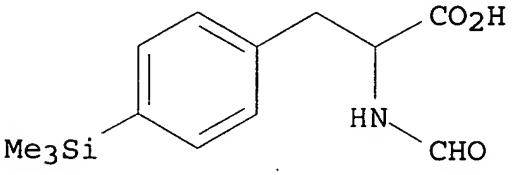
AB DL-p-Trimethylsilylphenylalanine has been prepared in good yield by condensation of 4-trimethylsilylbenzyl bromide with diethyl formamidomalonate, followed by mild hydrolysis and **decarboxylation** of the resulting disodium α-(4-trimethylsilylbenzyl)formamidomalonate. Its N-carboxy anhydride was obtained on reaction of the amino acid with carbonyl chloride, and it has been **polymerized** in pyridine.

IT **15102-53-1**, Alanine, 3-[p-(trimethylsilyl)phenyl]-, DL-
18162-46-4, Alanine, N-formyl-3-[p-(trimethylsilyl)phenyl]-, DL- **18727-26-9**, Alanine, N-acetyl-3-[p-(trimethylsilyl)phenyl]-, DL-
(preparation of)

RN 15102-53-1 HCAPLUS
CN Phenylalanine, 4-(trimethylsilyl)- (9CI) (CA INDEX NAME)

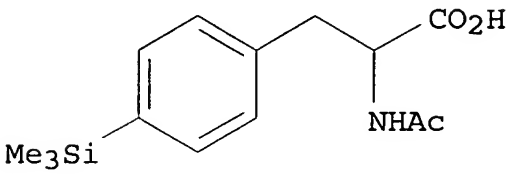


RN 18162-46-4 HCAPLUS
CN Alanine, N-formyl-3-[p-(trimethylsilyl)phenyl]-, DL- (8CI) (CA INDEX NAME)



RN 18727-26-9 HCAPLUS

CN Alanine, N-acetyl-3-[p-(trimethylsilyl)phenyl]-, DL- (8CI) (CA INDEX NAME)



CC 44 (Amino Acids, Peptides, and Proteins)
IT **Polymerization**
(of 4-[p-(trimethylsilyl)benzyl]-2,5-oxazolidinedione)
IT Spectra, **infrared**
(of 4-[p-(trimethylsilyl)benzyl]-2,5-oxazolidinedione and related compds.)
IT 3728-43-6, Silane, trimethyl-p-tolyl- **15102-53-1**, Alanine, 3-[p-(trimethylsilyl)phenyl]-, DL- 17938-42-0, Malonic acid, acetamido[p-(trimethylsilyl)benzyl]- 17938-55-5, Malonic acid, acetamido[p-(trimethylsilyl)benzyl]-, disodium salt 18052-63-6, 2,5-Oxazolidinedione, 4-[p-(trimethylsilyl)benzyl]- **18162-46-4**, Alanine, N-formyl-3-[p-(trimethylsilyl)phenyl]-, DL- 18410-22-5, Malonic acid, formamido[p-(trimethylsilyl)benzyl]-, disodium salt 18677-02-6, Malonic acid, acetamido[p-(trimethylsilyl)benzyl]-, diethyl ester, (±)- **18727-26-9**, Alanine, N-acetyl-3-[p-(trimethylsilyl)phenyl]-, DL- 18862-75-4, Malonic acid, formamido[p-(trimethylsilyl)benzyl]-, diethyl ester, (±)-
(preparation of)

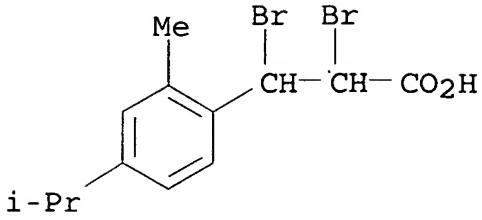
L128 ANSWER 47 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1963:20501 Document No. 58:20501 Original Reference No. 58:3342d-h
p-Cymene and its derivatives. XXXV. Friedel-Crafts acylation with p-cymene and reactions of 1-methyl-4-isopropyl-2-cinnamic acid.
Strubell, Wolfgang; Baumgaertel, Horst (VEB Deut. Hydrierwerk, Rodleben, Germany). Journal fuer Praktische Chemie (Leipzig), 17, 326-30 (Unavailable) 1962. CODEN: JPCEAO. ISSN: 0021-8383.
AB cf. ibid. 18, 113(1962); CA 57, 13657d. Friedel-Crafts acylation of p-cymene (I) with aliphatic acyl chlorides and with BzCl led to the corresponding phenones. Mannich reaction of the acetophenone derivative
with Me2NH yielded a compound with low anesthetic activity. Conversion of 1-methyl-4-isopropyl-2-cinnamic acid (II) to 2-vinyl-p-cymene (III) yielded a monomer that could be

polymerized to glass-clear block polymers. Thus 37.5 g. Ac2O were added over 45 min. with stirring to a mixture of 258 cc. I (dried over Na) and 120 g. AlCl3. After stirring 1 hr., unreacted AcOH and I were distilled to 190°, the residue steam-distilled, the product extracted with Et2O and distilled to give 5-isopropyl-2-methylacetophenone (IV), b12 124-6°. A mixture of 201 g. I, 107 g. isobutyryl chloride, and 35 g. AlCl3, after stirring 3 hrs. at 50°, was quenched in ice-H2O, dried, and the product distilled several times under vacuum to give 5'-isopropyl-2,2'-dimethylpropiophenone, b14 143°. Similarly, I and isovaleryl chloride gave 5'-isopropyl-2',3-dimethylbutyrophenone, b13 169-70°, b760 272°, and I and BzCl gave 5-isopropyl-2-methylbenzophenone, m. 56°, b755 305-8°. Reaction of 14 g. phthalic anhydride, 100 g. dry I, and 15 g. AlCl3 gave o-(5-isopropyl-2-methylbenzoyl)benzoic acid, m. 124°, which underwent **dehydrative** ring-closure with P2O5 to give 1-isopropyl-5-methyl-9,10-anthraquinone, m. 114° (C6H6). A mixture of 58.8 g. IV, 10 g. paraformaldehyde, and 27.5 g. Me2NH.HCl was boiled 6 hrs. in 50 cc. absolute EtOH. The reaction product was treated with Me2CO and cooled to near 0° to give a flocculent precipitate of 3-dimethylamino-5'-isopropyl-2'-methylpropiophenone-HCl, m. 181°. **Decarboxylation** of II followed by steam-, then vacuum-distillation, gave III, b15 61°. Treatment of III with 0.5% Bz2O2 at 70° gave a glass-clear block, slightly yellow by transmitted light. Halogenation of 0.5 mole II with Br at 100° to saturation required 165 g. Br. The Et2O extract of the reaction product deposited crystals of 2,3-dibromo-3-(5-isopropyl-2-methylphenyl)propionic acid (V), m. 216° (CHCl3) (decomposition). Dehydrohalogenation of 0.5 mole V with 50 g. KOH in boiling absolute EtOH 6 hrs., filtration, cooling, and treatment with dilute HCl until precipitation was complete gave 3-(5-isopropyl-2-methylphenyl)propynoic acid, m. 154°.

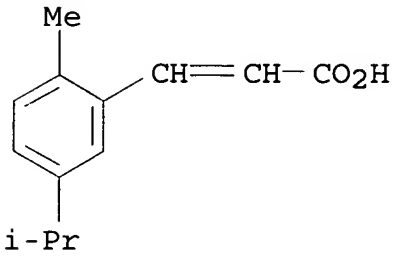
IT **767331-57-7**, m-Cymene-6-propionic acid, α,β-dibromo-
(preparation of)

RN 767331-57-7 HCAPLUS

CN m-Cymene-6-propionic acid, α,β-dibromo- (7CI) (CA INDEX NAME)



IT **4395-83-9**, p-Cymene-2-acrylic acid
(reactions of)
RN 4395-83-9 HCAPLUS
CN 2-Propenoic acid, 3-[2-methyl-5-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)



CC 35 (Noncondensed Aromatic Compounds)
IT 99-87-6, p-Cymene 1202-08-0, Acetophenone, 5'-isopropyl-2'-methyl- 38338-63-5, Styrene, 5-isopropyl-2-methyl- 64298-32-4, Butyrophenone, 5'-isopropyl-2',3-dimethyl- 91909-48-7, p-Cymene-2-propiolic acid 92300-56-6, Propiophenone, 5'-isopropyl-2,2'-dimethyl- 92725-79-6, Propiophenone, 3-(dimethylamino)-5'-isopropyl-2'-methyl-, hydrochloride 93651-28-6, Benzophenone, 5-isopropyl-2-methyl- 93875-31-1, Anthraquinone, 1-isopropyl-4-methyl- 93877-73-7, Benzoic acid, o-(5-isopropyl-o-toluoyl)- **767331-57-7**, m-Cymene-6-propionic acid, α,β-dibromo-
(preparation of)
IT **4395-83-9**, p-Cymene-2-acrylic acid
(reactions of)

L128 ANSWER 48 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1963:3422 Document No. 58:3422 Original Reference No. 58:561e-h,562e-h,563a Ozonolysis of conjugated systems. II. Cleavage of 17β-propionyloxy-1,4-androstadien-3-one. Caspi,

E.; Khan, B. Taqui; Balasubrahmanyam, S. N. (Worcester Found. Exptl. Biol., Shrewsbury, MA). Tetrahedron, 18, 1013-18 (Unavailable) 1962. CODEN: TETRAB. ISSN: 0040-4020.

GI For diagram(s), see printed CA Issue.

AB cf. CA 57, 13817e. The title compound (I, 6.92 g.) in 160 ml. EtOAc ozonized 7 hrs. at -70° (with disappearance of the ultraviolet absorption band at 240 mμ and appearance of a new maximum at 224 mμ) and the solution stirred 16 hrs. at 20° with 40 ml. H2O, the organic phase partitioned to give 5.49 g. neutral and 1.56 g. acidic fractions and the neutral fraction crystallized from EtOAc gave 450 mg. 17β-propionyloxy-5α-hydroxy-4-oxa-1-androsten-3-one (II, R = H, R' : EtCO) (III), m. 187-8°. The mother liquor concentrated chromatographed on silica **gel** and eluted with C6H6-CHCl3 mixts. gave 3.36 g. semisolid and 280 mg. 17β-propionyloxy-1α-hydroxy-2-oxa-4-androsten-3-one (IV). The semi-solid rechromatographed on silica **gel** gave 1.39 g. non-crystalline residue and 926 mg. III. The eluates were recombined and partitioned via aqueous Na2CO3 into 930 mg. V (R' : EtCO, R : H) (VI), m. 140-6°, and 380 mg. neutral semi-solid. The 1.56 g. acidic fraction gave III as the only identifiable production chromatography. Recrystn. from EtOAc-MeOH gave III, m. 187-8°, λ 217 mμ (ε 8000), ν 3450, 3020, 1750, 1700, 1630, 1195 cm.-1 [α]500235 [α]400 497°, [α]300 1762° (c 0.37, 27°, dioxane). III (40 mg.) in 3 ml. MeOH, 1.5 ml. 1.0N NaOH, and 3 ml. H2O boiled (N atmospheric) 2.5 hrs. and the MeOH removed in a stream of N, the alkaline solution washed with EtOAc and acidified gave 31 mg. lactol, twice recrystd. from EtOAc to give II (R = R' : H) (VII), m. 265-8°, λ 217 mμ (ε 8000), ν 3450, 3250, 1710, 1615, 1055 cm.-1 (KBr). III (50 mg.) refluxed 2 hrs. in 20 ml. redistd. Ac2O under N and the mixture refluxed 2 hrs. with 20 mg. freshly fused NaOAc, the residue on evaporation taken up in EtOAc, and the washed and dried extract concentrated gave 48.2 mg. residue, recrystd. twice from EtOAc-Et2O to give II (R : Ac, R' : EtCO) (VIII), m. 203-4°, λ 217 mμ (ε 8000), ν 1755, 1730, 1620, 1230 cm.-1 (KBr). VII (56 mg.) refluxed (N atmospheric) 4 hrs. in 30 ml. freshly distilled Ac2O and the product crystallized from EtOAc-CH2Cl2 gave II (R : R' = Ac) (IX), m. 129-30°, λ 217 mμ

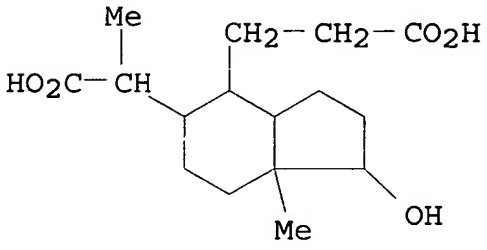
(ε 8000), ν 1750, 1630, 1250, 1225 cm.-1 III in MeOH treated with excess CH_2N_2 in Et_2O and the residue on evaporation crystallized from Et_2O-C_6H_{14} gave II (R : Me, R' : EtCO), m. 94°, λ 217 mμ (ε 7400), ν 1725, 1640, 1220 cm.-1 Similarly, 72 mg. VII in 5 ml. MeOH treated with CH_2N_2 in Et_2O gave II (R : Me, R' : H), m. 58° (Et_2O-C_6H_{14}), λ 217 mμ (ε 8400), ν 3450, 1715, 1695, 1625, 1175 cm.-1 (KBr). VIII (20 mg.) boiled 2.5 hrs. under N in 3 ml. MeOH and 1 ml. N NaOH gave VII, also produced by similar treatment of IX. III (48 mg.) in 6 ml. EtOAc hydrogenated 1 hr. with 55 mg. 10% Pd-C and the mixture filtered through Celite, the sirup on evaporation boiled (N atmospheric) 2 hrs. in 5 ml. MeOH with 2 ml. 2N NaOH, and the acid recovered in the conventional manner with EtOAc yielded 17β-hydroxy-5,5-seco-4-nor-5-androstanon-3-oic acid, also obtained by boiling 20 mg. 17-benzoyloxy-3,5-seco-4-nor-5-androstanon-3-oic acid in 5 ml. MeOH and 2 ml. 2N NaOH under N 2 hrs. Recrystn. from EtOAc-C_6H_{14} gave IV, m. 206-7°, λ 228 mμ (ε 13,000, MeOH), ν 3450, 1720, 1695, 1620, 1260, 1225 cm.-1 (KBr). Recrystn. from dilute MeOH yielded VI, m. 151-2°, ν 3400, 2900, 1730, 1695, 1190, 1035 cm.-1, n.m.r.) 5.35, 7.58, 7.67, 7.83, 8.75, 8.86, 8.98, 9.21 τ, $[\alpha]_{450}$ 84°, $[\alpha]_{350}$ 153°, $[\alpha]_{275}$ 483° (c 0.57 at 27°, dioxane), acid equivalent 302. The data indicated that VI was not the β-oxo acid (X, R : OH) and this was confirmed by recovery of unchanged starting material on boiling 40 mg. VI 4.5 hrs. in 3:5 H_2O-AcOH containing 0.4 ml. N H_3PO_4. VI (75 mg.) in 5 ml. 4:1 AcOH-2N HCl refluxed (N atmospheric) 2 hrs. and the volatile components evaporated in vacuo, extracted with EtOAc and the product (66 mg.) recrystd. from EtOAc gave V (R : R' : H), m. 189-90°, ν 3330, 2620, 1795, 1240 cm.-1 (KBr), n.m.r. 6.34, 8.88, 9.28 τ. III (250 mg.) in 20 ml. EtOAc ozonized at -70° until the band at 217 mμ disappeared, the solution stirred 16 hrs. at 20° with H_2O, and the products partitioned with aqueous $NaHCO_3$ gave 120 mg. aldehyde X (R : H), m. 125-6° (EtOAc-Et_2O), ν 2720, 1745, 1695, 1200 cm.-1 (KBr), and 132 mg. 1-propionyloxy-5-(α-carboxyethyl)- 4-(β-carboxyethyl)-8-methylhydrindane (XI), m. 110-11° (Et_2O-C_6H_{14}), ν 3100, 2700, 1745, 1710, 1280, 1200 cm.-1, n.m.r. 5.93, 7.88, 8.00, 8.17, 8.92, 9.01, 9.12, 9.29 τ, acid equivalent 189. For further evaluation of the intensities of the bands of the n.m.r. spectrum it was considered advantageous to remove the interfering propionate moiety. XI (4.3 mg.) refluxed 1 hr. (N atmospheric) in 1 ml. MeOH with 0.2

ml. 2N NaOH and the solution acidified with AcOH, the residue on evaporation
taken up in EtOAc, and the H2O-washed solution evaporated gave 3.8 mg. glassy material, ν 3400, 3160, 2650, 1695, 1200 cm.-1, n.m.r. 6.34, 8.73, 8.75, 8.83, 8.88, 9.24, τ, thus providing evidence for the assigned structure. A tentative mechanism for the rearrangements was proposed.

IT **94207-73-5**, 4-Indanpropionic acid, 5-(1-carboxyethyl)hexahydro-1-hydroxy-7a-methyl- **94441-64-2**, 4-Indanpropionic acid, 5-(1-carboxyethyl)hexahydro-1-hydroxy-7a-methyl-, propionate
(preparation of)

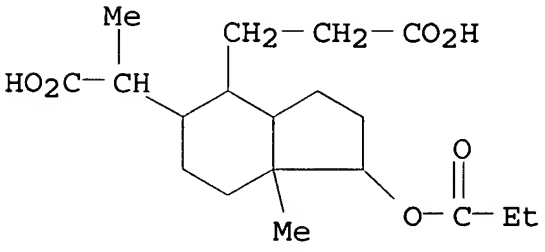
RN 94207-73-5 HCAPLUS

CN 4-Indanpropionic acid, 5-(1-carboxyethyl)hexahydro-1-hydroxy-7a-methyl- (7CI) (CA INDEX NAME)



RN 94441-64-2 HCAPLUS

CN 4-Indanpropionic acid, 5-(1-carboxyethyl)hexahydro-1-hydroxy-7a-methyl-, propionate (7CI) (CA INDEX NAME)



CC 42 (Steroids)

IT Nuclear magnetic resonance
Spectra, **infrared**
Spectra, visible and ultraviolet
(of 17β-hydroxyandrosta-1,4-dien-3-one propionate ozonolysis

products)
IT 545-84-6, Voacristine
(**decarboxylation** of)
IT 94198-60-4, 4-Oxa-5α-androst-1-en-3-one, 5,17β-dihydroxy- **94207-73-5**, 4-Indanpropionic acid, 5-(1-carboxyethyl)hexahydro-1-hydroxy-7a-methyl- **94441-64-2**, 4-Indanpropionic acid, 5-(1-carboxyethyl)hexahydro-1-hydroxy-7a-methyl-, propionate 94866-04-3, 4-Oxa-5α-androst-1-en-3-one, 17β-hydroxy-5-methoxy- 95562-90-6, 4-Oxa-5α-androst-1-en-3-one, 5,17β-dihydroxy-, 5-acetate 17-propionate 96066-69-2, 4-Oxa-5α-androst-1-en-3-one, 17β-hydroxy-5-methoxy-, propionate 98804-78-5, as-Indacene-3-carboxylic acid, dodecahydro-6-hydroxy-3,5a-dimethyl-, propionate 100228-04-4, 4-Oxa-5α-androst-1-en-3-one, 5,17β-dihydroxy-, diacetate 104781-39-7, 1H-Benz[e]indene-6-carboxaldehyde, dodecahydro-3-hydroxy-3a,6-dimethyl-7-oxo-, propionate 105564-74-7, 1,5-Seco-A-trinorandrostan-1-al, 17β-hydroxy-5-oxo-, propionate 856774-11-3, 1H-Benz[e]indene-6-acrylic acid, 2,3,3a,4,5,5a,6,7,8,9,9a,9b-dodecahydro-3-hydroxy-3a,6-dimethyl-7-oxo-, methyl hemiacetal, δ-lactone, propionate 856774-14-6, 1H-Benz[e]indene-6-acrylic acid, 2,3,3a,4,5,5a,6,7,8,9,9a,9b-dodecahydro-3-hydroxy-3a,6-dimethyl-7-oxo-, methyl hemiacetal, δ-lactone
(preparation of)

L128 ANSWER 49 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1962:469415 Document No. 57:69415 Original Reference No. 57:13817c-i,13818c-i,13819a-g Ozonolysis of conjugated systems. I. Cleavage of steroidal Δ1,4-dien-3-ones in the C19O3 and C21lO5 series. Caspi, E.; Schmid, W.; Khan, B. Taqui (Worcester Found. Exptl. Biol., Shrewsbury, MA). Tetrahedron, 18, 767-75 (Unavailable) 1962. CODEN: TETRAB. ISSN: 0040-4020. OTHER SOURCES: CASREACT 57:69415.
AB cf. CA 56, 10215b. Ozonolysis of Δ1.4-oxo steroids gave products with partial or complete degradation of the cross-conjugated group. EtOAc (250 ml.) containing 5.0 g. 1,4-androstadiene-3,11,17-trione (I) was ozonized at -70° until the ultraviolet band at 238 mμ disappeared and the product rapidly distilled in H2O in vacuo, the residue taken up in EtOAc and partitioned with saturated aqueous NaHCO3 into 2.6 g. acidic fraction (II)
and 2.6 g. neutral fraction, crystallized from EtOAc to yield a small amount of material (III), m. 259-61°. The mother liquor from III chromatographed on silica **gel** and eluted with 1:49 EtOAc-CHCl3 gave 793 mg. aldehyde (IV). Further elution with 1:9

through 3:17 and with 1:4 through 3:7 EtOAc-CHCl3 gave 337 mg. lactol (V) and 220 mg. lactol (VI). II and 1 ml. 1.0N H3PO4 refluxed (N atmospheric) 2.5 hrs. in 60 ml. 1:1 AcOH-H2O with evolution of CO2 and the residue on evaporation partitioned gave 380 mg. neutral fraction containing 66 mg. trione (VII) and a small amount of V, and 2.21 g. acidic fraction, chromatographed on silica **gel** to give more V. VI recrystd. 3 times from EtOAc-MeOH yielded pure 1α-hydroxy-2-oxa-4-androstene3,11,17-trione, m. 259-61°, nuclear magnetic resonance 4.08, 4.37, 8.71, 9.22 τ, unchanged by treatment in Me2CO with CrO3-H2SO4 and with CrO3-C5H5N. VI (35 mg.) refluxed 2.5 hrs. in 15 ml. freshly distilled Ac2O and the mixture refluxed 2 hrs. with 20 mg. freshly fused NaOAc, the Ac2O evaporated in vacuo and the residue taken up in EtOAc, the washed and dried solution concentrated, and the product crystallized from AcOEt-CH2Cl2 (Norit) gave 1α-acetoxy-2-oxa-4-androstene-3,11,17-trione, m. 216-17°, also produced by acetylation with Ac2O-C5H5N 12 hrs. at 20°. VI (30 mg.) in 5 ml. MeOH kept 1 hr. at 20° with excess CH2N2 in Et2O, the volatile components removed in a stream of N, and the material recrystd. 3 times from EtOAc-MeOH gave pure Me 1,3-seco-2-norandrost-4-ene-11,17-dion-1-al-3-carboxylate, m. 179-80°. IV [70 mg., m. 157-8° (EtOAc)] in 4 ml. EtOAc ozonized at - 70° and the blue solution kept 16 hrs. at - 70°, diluted with 20 ml. H2O and stirred 30 min. at 20°, the aqueous phase extracted with EtOAc, and the combined layers partitioned with NaHCO3 gave 60 mg. acid, twice recrystd. from EtOAc to give 1,5-seco-2,3,4-trinorandrostane-5,11,17trione-1-carboxylic acid (VIII), m. 131-2°. VIII (40 mg.) and 2-3 drops 1.0N H3PO4 refluxed (N atmospheric) 2 hrs. in 3.0 ml. 1:1 H2O-AcOH and the volatile components evapd, in vacuo, the residue taken up in EtOAc, and the washed (saturated aqueous NaHCO3, saturated aqueous NaCl) and dried solution concentrated gave 34 mg. triketone, repeatedly recrystd. from EtOAc to give 5,10-seco-1,2,3,4-tetranorandrostane-5,11,17-trione, VII, m. 135-7°. V, m. 219-20° (EtOAc-MeOH), esterified with excess CH2N2 in Et2O gave Me 3,5-seco-4-nor-1-androstene-5,11,17-trione-3-carboxylate. V, 5α-hydroxy-4-oxa1-androstene-3,11,17-trione (30 mg.) in 5 ml. 4:1 EtOAc-MeOH hydrogenated 45 min. at 20° with 50 mg. Pd-C and the filtered solution evaporated gave authentic 3,5-seco-4-nor- androstane-5,11,17-trione-3-carboxylic acid. Ozonization of 1-dehydrocorticosteroids was studied by an

investigation of the ozonization products of prednisone 21-acetate (IX). IX (400 mg.) in EtOAc was ozonized at - 70° to disappearance of the 240 mμ band and the mixture rapidly distilled with 4 ml. H2O, the residue repeatedly diluted with H2O and recovered, the product taken up in EtOAc and partitioned into 295 mg. neutral and 130 mg. acidic fractions. Crystallization of the neutral fraction gave 90 mg. aldehyde (X) and a small amount of acetate (XI). The acidic fractions (830 mg. from several runs) and 3 ml. 1.0N H3PO4 refluxed (N atmospheric) 2 hrs. in 30 ml. AcOH, the AcOH removed in a stream of N, and the residue taken up in EtOAc and partitioned gave 54 mg. neutral acetate (XII). X repeatedly crystallized from EtOAc yielded 21-acetoxy-17α-hydroxy-1,5-seco-2,3,4-trinorpregnane-5,11,20-trion-1-al, m. 192-5°, also produced by ozonization of prenisolone acetate. The mother liquors from X gave a small amount of XI, recrystd. from MeOH-CH2Cl2 to give crystalline 21-acetoxy-1α,17α-dihydroxy-2-oxa-4-pregnene-3,11,20-trione, m. 260-5°. X (200 mg.) in 10 ml. EtOAc saturated with ozone at -70° and stored 16 hrs. at -70°, partitioned with NaHCO3, and the crystalline acidic fraction (152 mg.) recrystd. from EtOAc gave 21-acetoxy-17α-hydroxy-1,5-seco-2,3,4-trisnorpregnane-5,11,20-trione1-carboxylic acid, m. 119-21° (resolidified and m. 171-7°), **decarboxylated** by refluxing in alc. with 0.1N H3PO4 to give 21-acetoxy-17α-hydroxy-5,10-seco-1,2,3,4-tetranorpregnane-5,11,20-trione, m. 179-82° (EtOAc), [α]D 122° (c. 0.72, MeOH), [α]D 137° (c 0.72, CHCl3), also obtained by **decarboxylation** of the combined acidic residues of several ozonizations of IX. The acetate (105 mg.) kept (N atmospheric) 16 hrs. at 20° in 8 ml. 1:1 MeOH-H2O with 120 mg. Na2CO3 and the mixture acidified with 2N HCl, the MeOH removed in a stream of N and the residue taken up in EtOAc, chromatographed on silica **gel**, and the eluate evaporated gave 33 mg. 17α,21-dihydroxy-5,10-seco-1,2,3,4-tetranorpregnane-5,11,20-trione, m. 167-8°. The sequence of reactions constituted conclusive proof of the assigned structures of X and XII. The structure assigned to XI was confirmed by an independent procedure. Prednisone-4-C14 21-acetate (XIII) was prepared by SeO2 or microbiol, dehydrogenation of cortisone-4-C14 21-acetate (XIV). Erlenmeyer flasks containing 100 ml. 1% yeast extract broth inoculated with Bacillus sphaericus agitated 24 hrs. at 37° and 25 mg. XIV (sp. activity 250 + 103 counts/min./millimole) in a min. amount of alc. added, incubation of a

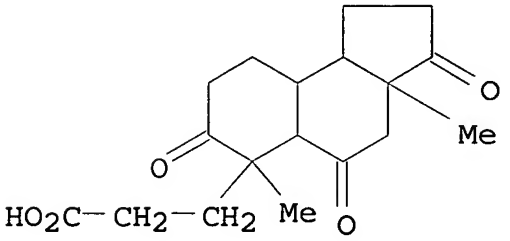
total 800 mg. XIV continued 24 hrs. and the steroids recovered with CHCl3, the extract chromatographed on silica **gel**, and the fractions evaporated gave 568 mg. I-4-C14 and only 50.9 mg. XIII (sp. activity 246 + 103 counts/min./millimole). XIV (285 mg., sp. activity 125 + 103 counts/min./millimole) in 15 ml. Me3COH and 0.15 ml. AcOH refluxed 7 hrs. with 90 mg. SeO2, the mixture refluxed 12 hrs. with 90 mg. addnl. SeO2 and the cooled, filtered solution concentrated, the residue taken up in EtOAc and the washed (H2O, aqueous NaHCO3) and dried solution concentrated, the concentrate refluxed 1 hr. with 86 mg. precipitated Ag, and the filtered solution decolorized (Norit) and evaporated, the residue chromatographed and the impure active product (41 mg.) diluted with 163 mg. non-radioactive IX gave slightly colored XIII, sp. activity 19.0 + 103 counts/min./mole. Erlenmeyer flasks containing 100 ml. 0.1% yeast extract broth inoculated with A rthrobacter simplex agitated 24 hrs. at 37°, treated with 25 mg. cortisone-C14 in a min. of HCONMe2 and incubated 24 hrs., extracted with CHCl3 and the extract from 310 mg. steroid chromatographed on silica **gel** gave 194 mg. prednisone-C14, acetylated with Ac2O-C6H5N to yield 210 mg. XIII. XIII (350 mg., sp. activity 55.2 + 103 counts/min./millimole) in 30 ml. EtOAc ozonized at -70° and processed as above gave 117 mg. neutral fraction, crystallized from EtOAc to yield 7.6 mg. XI, sp. activity 55 + 103 counts/min./millimole, and 56.8 mg. X with no activity in agreement with the assigned structures. Analogous results were obtained with prednisone bis(methylene dioxide) (XV). XV (1 g.) ozonized in 50 ml. EtOAc at -70° and processed as described yielded 531 mg. 1,5-seco-2,3,4-trinorpregnane-5,11-dion-1-al-17,20:20,21-bis(methylene dioxide), m. 236-40°. The aldehyde treated with ozone in 25 ml. EtOAc at -70° and the products partitioned gave 67 mg. neutral residue and 123 mg. 1,5-seco-2,3,4-trinorpregnane-5,11-dione-1-carboxylic acid 17,20:20,21-bis(methylene dioxide), m. 130-4°. The assumption was made that the lactol V will have the less strained configuration with the 3,5-oxa bond junction in the 5β position, and that the lactol rings of VI and XI will assume a pseudo chair form and the C-1 OH the α-configuration, thus minimizing possible interaction between the OH and the angular Me groups. Ultra-violet and **infrared** spectral data were given.

IT **98706-00-4**, 1H-Benz[e]indene-6-propionic acid, dodecahydro-3a,6-dimethyl-3,5,7-trioxo- **98843-09-5**,

3,5-Seco-A-norandrostan-3-oic acid, 5,11,17-trioxo-
(preparation of)

RN 98706-00-4 HCAPLUS

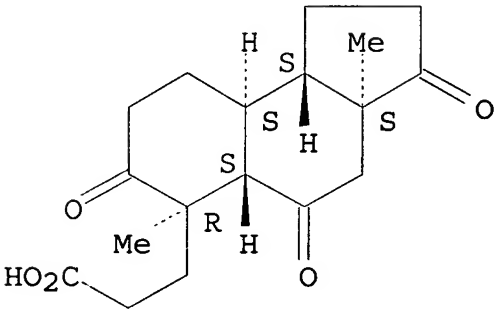
CN 1H-Benz[e]indene-6-propionic acid, dodecahydro-3a,6-dimethyl-3,5,7-trioxo- (7CI) (CA INDEX NAME)



RN 98843-09-5 HCAPLUS

CN 3,5-Seco-A-norandrostan-3-oic acid, 5,11,17-trioxo- (7CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 36 (Steroids)

IT Spectra, **infrared**
Spectra, visible and ultraviolet
(of 3-keto Δ1,4-steroid ozonolysis products and their derivs.)

IT 94686-97-2, 2-Oxaandrost-4-ene-3,11,17-trione, 1α-hydroxy-, acetate 95316-26-0, 2-Oxaandrost-4-ene-3,11,17-trione, 1α-hydroxy- 95316-27-1, 4-Oxa-5α-androst-1-ene-3,11,17-trione, 5-hydroxy- 96587-73-4, 2-Oxapregn-4-ene-3,11,20-trione, 1α,17,21-trihydroxy-, 21-acetate 97499-29-1, 1H-Benz[e]indene-6-carboxaldehyde, dodecahydro-3a,6-dimethyl-3,5,7-trioxo- 97525-69-4, 5,10-Seco-A-tetranorandrostane-5,11,17-trione

97554-27-3, 1,5-Seco-A-trinorandrostan-1-al, 5,11,17-trioxo- 97596-44-6, 1,5-Seco-A-trinorandrostan-1-oic acid, 5,11,17-trioxo- 97810-26-9, 3H-Benz[e]indene-3,5,7-trione, decahydro-3a,6-dimethyl- 98468-68-9, 1H-Benz[e]indene-5,7-dione, 3-glycoloyldecahydro-3-hydroxy-3a,6-dimethyl- **98706-00-4**, 1H-Benz[e]indene-6-propionic acid, dodecahydro-3a,6-dimethyl-3,5,7-trioxo- 98739-56-1, 5,10-Seco-A-tetranorpregnane-5,11,20-trione, 17,21-dihydroxy- **98843-09-5**, 3,5-Seco-A-norandrostan-3-oic acid, 5,11,17-trioxo- 99711-40-7, 1H-Benz[e]indene-6-carboxaldehyde, 3-glycoloyldodecahydro-3-hydroxy-3a,6-dimethyl-5,7-dioxo-, acetate 100302-93-0, 1H-Benz[e]indene-6-carboxylic acid, dodecahydro-3a,6-dimethyl-3,5,7-trioxo- 100625-58-9, Dispiro[3H-benz[e]indene-3,4'-[1,3]dioxolane-5',4''-[1,3]dioxolane]-6-carboxylic acid, dodecahydro-3a,6-dimethyl-5,7-dioxo- 100625-58-9, 1,5-Seco-A-trinorpregnan-1-oic acid, 17,20:20,21-bis(methylenedioxy)-5,11-dioxo- 100627-69-8, 1H-Benz[e]indene-6-carboxylic acid, 3-glycoloyldodecahydro-3-hydroxy-3a,6-dimethyl-5,7-dioxo-, acetate 102287-46-7, 5,10-Seco-A-tetranorpregnane-5,11,20-trione, 17,21-dihydroxy-, 21-acetate 102378-22-3, 1,5-Seco-A-trinorpregnan-1-al, 17,21-dihydroxy-5,11,20-trioxo-, 21-acetate 103591-91-9, 1H-Benz[e]indene-5,7-dione, 3-glycoloyldecahydro-3-hydroxy-3a,6-dimethyl-, acetate 104852-98-4, 3,5-Seco-A-norandrost-1-en-3-oic acid, 17β-hydroxy-17-methyl-5-oxo-, methyl ester 105583-91-3, 1,5-Seco-A-trinorpregnan-1-oic acid, 17,21-dihydroxy-5,11-20-trioxo-, 21-acetate 111211-57-5, Dispiro[3H-benz[e]indene-3,4'-[1,3]dioxolane-5',4''-[1,3]dioxolane]-6-carboxaldehyde, dodecahydro-3a,6-dimethyl-5,7-dioxo- 111211-57-5, 1,5-Seco-A-trinorpregnan-1-al, 17,20:20,21-bis(methylenedioxy)-5,11-dioxo- 856774-17-9, 1H-Benz[e]indene-6-acrylic acid, 2,3,3a,4,5,5a,6,7,8,9,9a,9b-dodecahydro-3a,6-dimethyl-3,5,7-trioxo-, methyl ester 856774-20-4, 7H-Benz[e]indene-Δ7,α-acetic acid, 6-formyldodecahydro-3a,6-dimethyl-3,5-dioxo-, methyl ester
(preparation of)

L128 ANSWER 50 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1962:12888 Document No. 56:12888 Original Reference No. 56:2393b-i,2394a-g An alternative synthetic approach to (±)-gibberone. Money, T.; Raphael, R. A.; Scott, A. I.; Young, D. W. (Univ. Glasgow, UK). Journal of the Chemical Society, Abstracts 3958-62 (Unavailable) 1961. CODEN: JCSAAZ. ISSN: 0590-9791.

AB The preparation was reported of 1,2,3,10-tetrahydro-2,8-di-methyl-3-oxofluorene-10-acetic acid (I), which was the key intermediate in the recent (Loewenthal, CA 55, 7376f) synthesis of (±)-gibberone,

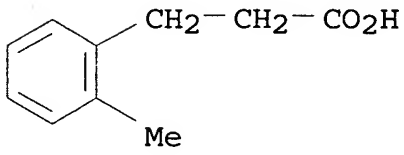
a transformation product of gibberellic acid. (**Infrared** spectra determined in CCl4 unless otherwise stated; ultraviolet spectra determined in EtOH; petr. ether used b. 60-80°; the phrase "in the usual way" implies diluting with H2O, extracting with Et2O, washing the extract with aqueous NaHCO3, dilute HCl, and H2O, drying, and concentrating in vacuo on a steam bath, and when necessary adding C6H6 or CHCl3 to remove final traces of H2O). 2-MeC6H4CH:-CHCO2H (20 g.) in 120 cc. 10% aqueous NaOH containing 3 g. 5% Pd-C shaken with H (1 mole equivalent H absorbed in 2 hrs.) gave 18.5 g. 2-MeC6H4CH2CH2CO2H (II), m. 102-4° (petr. ether). II (8 g.) and 150 g. polyphosphoric acid stirred 3 hrs. at 100°, the sirup added to 400 cc. H2O, and worked up in the usual way gave 5.5 g. 4-methyl-1-indanone (III), m. 98-101° (petr. ether). CH2:CHCN (2.2 g.) added at room temperature to 3 g. III in 30 cc. dry C6H6 containing 300 mg. Triton B and after 16 hrs. the solution worked up in the usual way gave crude CMe:CH.CH:CH.C:C.CH2-(CH2CH2R)2.CO (IV) (R = CN). Crude IV (R = CN) refluxed 8 hrs. with 100 cc. 10% aqueous KOH and the acidic fraction isolated gave 4.5 g. IV (R = CO2H), m. 160-4° (H2O), ν (Nujol) 1720 and 1700 cm.-1 IV (R = CO2H) refluxed 8 hrs. with EtOH and H2SO4, the crude ester (21.6 g.) added dropwise during 1 hr. with stirring to 175 cc. refluxing dry C6H6 containing 1.44 g. powdered Na, the mixture refluxed and stirred 12 hrs., cooled, treated with ice-cold dilute HCl, and worked up in the usual way gave 13.2 g. Et 4-methyl-1-oxoindan-2-spiro-1'-(4'-oxo-3'-cyclohexanecarboxylate) (V), m. 131-3° (EtOH), ν 1720, 1670, and 1615 cm.-1, λ 250-2 and 295-300 mμ (ε 26,200 and 3080). V (10 g.) in 40 cc. AcOH containing 10 cc. concentrated HCl and 6 cc. H2O refluxed 5 hrs. in N atmospheric, cooled, and added to 150 cc. ice H2O gave 7 g. 4-methyl-1-oxoindan-2-spiro-1'-(cyclohexan-4'-one) (VI), m. 123-6° (aqueous EtOH), ν 1720 cm.-1, λ 250-5 and 298 mμ (ε 12,700 and 2420). MeMgBr solution (prepared by adding 20 cc. MeBr in 25 cc. dry Et2O to 2 g. Mg in 10 cc. dry Et2O) treated dropwise with 4.6 g. VI in 100 cc. 1:1 Et2O-tetrahydrofuran with stirring while refluxing, after 3 hrs. the complex decomposed with 50 cc. saturated aqueous NH4Cl, and the mixture

worked up in the usual way gave 5.1 g. crude 1-hydroxy-1,4-dimethylindan-2-spiro-1'-(4'-methylcyclohexan-4'-ol) (VII), gum, ν 3400 and 1600 cm.-1, λ 265 mμ (ε 430). Crude VII (5.1 g.) in 150 cc. dry C6H6 containing 400 mg. p-MeC6H4SO3H refluxed 3 hrs. under a Dean and Stark apparatus, the solution processed in the usual way, the oily product (4.3 g.) chromatographed in petr. ether over Al2O3, and eluted with petr. ether gave 4-methyl-1-methyleneindan-2-spiro-1'-(4'-methylcyclohex-3'-ene) (VIII), m. 67-9° (petr. ether), ν 1635 and 1600 cm.-1, λ 255, 290, and 300 mμ (ε 15,500, 3940, and 3520). VIII (1 g.) in 50 cc. EtOAc ozonized 2 hrs. at -70°, the EtOAc removed in vacuo at 40°, the residue treated with 15 cc. AcOH containing 5 cc. 30% H2O2 and 2 drops dilute HCl, the solution kept 16 hrs. at room temperature, heated 10 min. on a steam bath, neutralized with aqueous NaHCO3, extracted with Et2O, acidified, and the product isolated with EtOAc gave 1 g. 4-methyl-1-oxo-2-(3-oxobutyl)-2-indanacetic acid (IX), oil, ν 1700 and 1600 cm.-1, converted with CH2N2 to the Me ester (X) of IX, oil, 1735 and 1715 cm.-1, λ 250 and 295 mμ (ε 7200 and 1400). X (800 mg.) in 100 cc. MeOH containing 1 g. Na refluxed 4 hrs. in a N atmospheric, the solution concentrated to 30 cc., treated with 75 cc. H2O, acidified with dilute HCl, extracted with EtOAc, the extract concentrated, and the residual oil (600 mg.) triturated with Et2O gave 250 mg. 1,2,3,10-tetrahydro-3-oxofluorene-10-acetic acid, amorphous, m. 218-25°; Me ester (XI), m. 109-11° (EtOAc-petr. ether). To 450 mg. NaOMe in 15 cc. dry C6H6 was added 600 mg. HCO2Et in 5 cc. dry C6H6, the mixture stirred 40 min. at room temperature under N, cooled in ice, treated with 1 g. XI in 35 cc. dry C6H6 at 0°, kept 30 min. at 0°, stirred overnight at room temperature, acidified with dilute H2SO4, and the product isolated with Et2O to give 900 mg. hydroxymethylene derivative (XII), oil, ν 1760, 1670, and 1640 cm.-1, λ 238 and 300 mμ (λ 7400 and 12,800), λ (0.1N alc.-NaOEt) 232, 295, and 390-5 mμ (ε 7900, 13,000, and 5150), purple with FeCl3. XII (900 mg.) in 25 cc. AcOH containing 900 mg. HONH2.HCl refluxed 25 min. under N, cooled, diluted with 200 cc. H2O, and worked up in the usual way gave 700 mg. crude isoxazole compound (XIII), oil, 1730 and 1630 cm.-1, λ 238 and 320 mμ (ε 7200 and 11,700), no

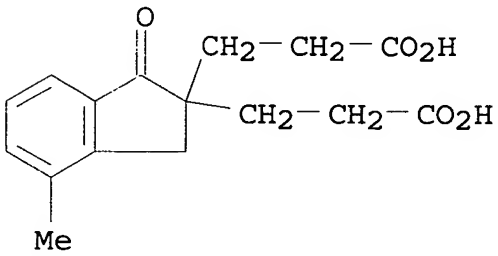
color with alc.-FeCl3. Crude XIII (700 mg.) in 5 cc. dry MeOH added under N to ice-cold NaOMe solution (from 150 mg. Na and 5 cc. dry MeOH), the solution kept 30 min. at room temperature, refluxed 10 min., cooled, treated with 1 cc. MeI, stirred 1 hr. at 20°, treated with 0.5 cc. MeI, refluxed 2 hrs., and worked up in the usual way gave 250 mg. Me 2-cyano-1,2,3,10-tetrahydro-2,8-dimethyl-3-oxofluoren-10-ylacetate (XIV), m. 191-5° (EtOAc), ν 2250, 1675, and 1640 cm.-1, λ 240 and 302-10 mμ (ε 8150 and 20,300). Attempted cyclization of XIV with tert-BuOK in tert-BuOH gave intractable products. To 100 mg. XII in 1.5 cc. dry HCONMe2 was added 30 mg. NaH, the mixture stirred 1.5 hrs. under N, treated with 0.7 cc. MeI under ice cooling, stirred 1 hr. at 0°, allowed to reach room temperature, stirred 4 hrs., worked up in the usual way, the resulting oil refluxed 3.5 hrs. in 5 cc. EtOH containing 1 cc. 60% aqueous KOH, extracted with Et2O, acidified, extracted with Et2O, the oily product triturated with iso-Pr2O, the resulting solid chromatographed in C6H6 on silical **gel**, and eluted with 19:1 C6H6-Et2O to give I, m. 169.5-70.0°, identical (mixed m.p., mass spectrum, and **infrared** spectrum) with authentic I. V (6 g.) in 30 cc. dry C6H6 added dropwise to 500 mg. powdered Na in 5 cc. dry C6H6 with stirring, the mixture stirred 30 min. at room temperature, refluxed 1 hr., cooled, treated with 2 cc. MeI, the whole refluxed 8 hrs., worked up in the usual way, the resulting oil (6 g.) refluxed 6 hrs. in 20 cc. AcOH containing 8 cc. concentrated HCl and 4 cc. H2O under N, and diluted with 120 cc. ice H2O gave 4 g. 4-methyl-1-oxoindan-2-spiro-1'-(3'methylcyclohexan-4'-one) (XV), m. 112-14° (aqueous MeOH), ν 1710 cm.-1, λ 252 and 299 mμ (ε 12,500 and 2300). XV was converted in the usual way with NaOH-EtOH to the crude furfurylidene derivative (XVI) of XV, oil, λ 250 and 325 mμ (ε 13,000 and 17,500). Crude XVI (600 mg.) ozonized 30 min. at -70° in 40 cc. EtOAc, the EtOAc removed, the residue oxidized in 5 cc. AcOH containing 2 cc. 30% H2O2 and 1 cc. dilute HCl, the acidic product isolated, and esterified gave 320 mg. oxo diester (XVII), oil, ν 1735 and 1700 cm.-1, λ 250 and 295 mμ (ε 1200 and 1800). XVII subjected to Dieckmann cyclization and the resulting oxo ester (ε 1720, 1665, and 1620 cm.-1) hydrolyzed and **decarboxylated** gave 4-methyl-1-oxoindan-2-spiro-1'-(4'-methylcyclopentan-3'-one), b0.4 140°, ν 1745 and 1715 cm.-1, λ 252 and 299 mμ (ε 12,300 and 2200).

IT **22084-89-5**, Hydrocinnamic acid, o-methyl- **93006-99-6**, 2,2-Indandipropionic acid (3,3'-(2-indanylidiene)dipropionic

acid), 4-methyl-1-oxo-
(preparation of)
RN 22084-89-5 HCAPLUS
CN Benzenepropanoic acid, 2-methyl- (9CI) (CA INDEX NAME)



RN 93006-99-6 HCAPLUS
CN 2,2-Indandipropionic acid, 4-methyl-1-oxo- (7CI) (CA INDEX NAME)



CC 30 (Condensed Aromatic Compounds)
IT Spectra, **infrared**
(of fluorene derivs. and spiro[cyclohexane-1,2'-indan] derivs.)
IT **22084-89-5**, Hydrocinnamic acid, o-methyl- 24644-78-8, 1-Indanone, 4-methyl- 92965-72-5, 2,2-Indandipropionitrile (3,3'-(2-indanylidene)dipropionitrile), 4-methyl-1-oxo- 93006-69-0, 2-Indanacetic acid, 4-methyl-1-oxo-2-(3-oxobutyl)- **93006-99-6**, 2,2-Indandipropionic acid (3,3'-(2-indanylidiene)dipropionic acid), 4-methyl-1-oxo- 93434-55-0, Fluorene-8a(6H)-acetic acid, 7,8-dihydro-1-methyl-6-oxo- 93728-19-9, 2-Indanacetic acid, 4-methyl-1-oxo-2-(3-oxobutyl)-, methyl ester 95279-61-1, Fluorene-8a(6H)-acetic acid, 7-cyano-7,8-dihydro-1,7-dimethyl-6-oxo-, methyl ester 97785-45-0, Spiro[cyclohexane-1,2'-indan]-1',4-dione, 3,4'-dimethyl- 98031-63-1, Fluorene-8a(6H)-acetic acid, 7,8-dihydro-7-methyl-6-oxo- 98031-84-6, Fluorene-8a(6H)-acetic acid, 7,8-dihydro-1-methyl-6-oxo-, methyl ester 98437-91-3, Spiro[cyclohexane-1,2'-indan]-3-carboxylic acid, 4'-methyl-1',4-dioxo-, ethyl ester 98692-83-2,

Spiro[3-cyclohexene-1,2'-indan], 4,4'-dimethyl-1'-methylene- 98738-57-9, Spiro[cyclohexane-1,2'-indan]-1',4-dione, 4'-methyl- 98739-42-5, Spiro[cyclopentane-1,2'-indan]-1',3-dione, 4,4'-dimethyl- 106480-20-0, Spiro[cyclohexane-1,2'-indan]-1',4-diol, 1',4,4'-trimethyl-
(preparation of)

L128 ANSWER 51 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1960:128423 Document No. 54:128423 Original Reference No. 54:24484c-h
Preparation and **polymerization** of p-vinylphenol. Sovish, Richard C. (Dow Chem. Co., Midland, MI). Journal of Organic Chemistry, 24, 1345-7 (Unavailable) 1959. CODEN: JOCEAH. ISSN: 0022-3263.

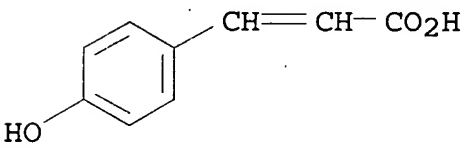
AB The direct synthesis of the title compound (I) was successfully carried out by the **decarboxylation** of p-HOC6H4CH:CHCO2H (II) by the **decarboxylation** procedure of Wiley and Hobson (CA 45, 3647a). H2C(CO2H)2 (104 g.) and 122 g. p-HOC6H4CHO in 150 ml. distilled C5H5N containing 5 ml. PhNH2 as catalyst gave by the method of Vorsatz (CA 30, 52021) 148 g. material, m. 206.8°, recrystd. 3 times from 1:3 MeOH.H2O to yield 41% II, m. 213.0-14.5°. II (82 g.) in 300 g. distilled quinoline added dropwise to 5 g. Cu powder in a 125 ml. Claisen flask at 225° in vacuo at a rate preventing accumulation of liquid and the distillate taken up in 150 ml. peroxide-free Et2O mixed with 200 g. crushed ice and stirred with slow addition of 1200 ml. cold 3N H2SO4, the Et2O and Et2O washings combined and the washed (ice-cold H2O) and dried (Drierite) Et2O evaporated in vacuo, the residue (44 g.) recrystd. at -15° from 500 ml. ligroine (b. 60-70°) to give 5 g. polymer (III) and 41% crystalline plates, m. 71-2.5°, recrystd. to give I, m. 72-3.5°, giving a blue color with FeCl3-concentrated HCl, titrated with standard bromate-bromide or Br-CCl4 solns. to give 4.09 and 4.07 added Br atoms per mole monomer. The same procedure but with extraction of the distillate with 10% aqueous NaOH and neutralization with acid or CO2 gave mainly III. I (5 g.) and 0.005 g. azobisisobutyronitrile (IV) heated 16 hrs. at 60° and the glassy solid taken up in MeCOEt, precipitated by pouring into C6H12 and repptd. gave 4.9 g. colorless powdery III, m. 229° (sintering at 207-15°). I (2.4 g.) and 18.72 g. H2C:CHPh heated 25 hrs. at 60° with 0.02 g. IV and repptd. twice from MeCOEt with C6H12 gave 4.0 g. copolymer, m. 164-98°, with approx. composition of 19 mole-% I. To observe the effects of various

catalysts, 1 g. I in 10 ml. MeCOEt was treated with BF3-Et2O in C6H12 and with AlCl3 in (Cl2CH)2 or I in C2H12 was treated with a small amount of H2SO4. The polymer was precipitated immediately and a blue color appeared which darkened on standing. I heated directly 24 hrs. at 60° with Bz2O2 also gave a polymer. All polymers were soluble in alc. and repptd. from H2O. Addition of I to 1:9 H2SO4-AcOH gave a purple solution with an immediate exothermic reaction. The solution darkened on keeping and increased markedly in viscosity to give an alc.insol. polymer also insol. in dioxane, Me2CO, and HCONMe2, although swellable and isolated by pouring the reaction mixture into H2O. **Infrared** spectra of I and III were charted.

IT **7400-08-0**, Cinnamic acid, p-hydroxy-
(preparation and **decarboxylation** of)

RN 7400-08-0 HCAPLUS

CN 2-Propenoic acid, 3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



CC 10E (Organic Chemistry: Benzene Derivatives)

IT **Polymerization**
(of p-vinylphenol)

IT **Infrared** spectra
(of p-vinylphenol polymers)

IT **7400-08-0**, Cinnamic acid, p-hydroxy-
(preparation and **decarboxylation** of)

IT 2628-17-3, Phenol, p-vinyl-
(preparation and **polymerization** of)

L128 ANSWER 52 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

1960:103145 Document No. 54:103145 Original Reference No. 54:19556i,19557a-g Claisen rearrangement. III. Benzyl 2-propenyl-4,6-dimethylphenyl ether. Marvell, Elliot N.; Dupzyk, Ronald Jene; Stephenson, John L.; Anderson, Richard (Oregon State Coll., Corvallis). Journal of Organic Chemistry, 25, 608-11 (Unavailable) 1960. CODEN: JOCEAH. ISSN: 0022-3263.

AB cf. CA 49, 5354f. The title compound (I) was synthesized and its behavior at temps. up to 210° was studied. At 135-50°, I started to **polymerize**, but showed no

tendency to form phenolic products. At 180-210°, the formation of phenolic materials was evident. One liquid phenolic compound was isolated and identified as 2-(2-benzylpropyl)-4,6-dimethylphenol (II). This identification was confirmed by synthesis. A 49% yield of 2-propenyl-4,6-dimethylphenol (III) was obtained in a 3 step synthesis from 2,4-dimethylphenol, m. 72-3°. NaOMe (from 7.1 g. Na in 150 ml. MeOH) and 50 g. III treated during 20 min. under reflux with 39 g. benzyl chloride, the mixture refluxed 3 hrs., cooled, mixed with ligroine, and extracted with Claisen alkali, the ligroine solution dried, and evaporated gave 70.5 g. I; the crude I was distilled in a Hickman mol. still at 70-80°/10-6 mm. The distillate chromatographed on Al2O3 and again distilled gave I, ν 696, 732, 856, 973, 1217, 1378, and 1648 cm.-1, n25D 1.5710, γ 252 mμ, ε 11,300. The material was hydrogenated over 10% Pd-C in AcOH with absorption of 2 moles H, the solvent evaporated, the product taken up in ligroine, washed, and the resulting phenolic material extracted with 6N NaOH to yield, after acidification and extraction, 2-propyl-4,6-dimethylphenol, b1.5 90-5°, n25D 1.5193. I refluxed 8 hrs. at 0.01 mm. gave a viscous deep red material showing no absorption at 3200-3600 cm.-1 Another sample (14.59) of I was heated in the dark under O free N 6 hrs. at 200-10°, the 12 g. of residual material taken up in ligroine, extracted with 6N NaOH, followed by Claisen alkali, each of the combined exts. acidified, extracted with ligroine, and the solvent evaporated There was no product from the 6N NaOH extract and 2.8 g. clear viscous liquid, b0.15 132-4°, n22D 1.5570, ν 698, 738, 859, 1375, 1490, 1605, and 3600 cm.-1 From the original ligroine solution, 9.2 g. neutral polymer was recovered. α-Methyldihydrocinnamic acid (IV) was prepared by the conventional alkylation of di-Et methylmalonate with PhCH2Cl, basic hydrolysis in 80% aqueous alc., and **decarboxylation** at 180-200°. The yield was 62%, b8 150-2°, d22 1.0644, n21D 1.5142. IV (44 g.) treated 14 hrs. at 40° with 64 g. SOCl2, refluxed 2 hrs., and distilled gave 47.2 g. acid chloride (V), b10 116-17°, n22D 1.5162. 2,4-Dimethylphenol (85.5 g.) in 1 l. C6H6 treated dropwise during 1 hr. with 118 g. V, the mixture refluxed 3 hrs., washed with H2O and dilute NaHCO3, dried, and distilled gave 2,4-dimethylphenyl α-methyldihydrocinnamate (VI), b0.5 146-7°, n23D 1.5872, d2623 1.0437, ν 1760 cm.-1 VI (107 g.) and 160 g. AlCl3

left 20 hrs. at room temperature, warmed 2 hrs. with stirring, and the product hydrolyzed gave 43 g. 2-(1-oxo-2-benzylpropyl)-4,6-dimethylphenol (VII), m. 67-7.5° (90% alc.), ν 1640 cm.-1 VII (11 g.) added dropwise to 0.9 g. LiAlH4 in 200 ml. Et2O, the mixture poured into 10% H2SO4, the Et2O layer separated, and evaporated gave 4.7 g. 2-(1-hydroxy-2-benzylpropyl)-4,6-dimethylphenol (VIII), m. 157-8°. This isomer showed 2 partly overlapping bands in the OH stretching region at 3360 and 3480 cm.-1 The low-melting isomer, obtained in 3.1 g. yield, m. 104-6°, ν 3600 and 3360 cm.-1 VIII (1.2 g.) and 1.5 g. freshly fused KHSO4 heated 0.5 hr. at 160-70° and the product isolated by extraction with Et2O gave 0.96 g. 2-(2-benzylpropenyl)-4,6-dimethylphenol (IX), b0.15 124-5°, n21D 1.5795, d2523 1.0267. Similar **dehydration** of VIII (m. 104-6°) gave 96% IX. IX in AcOH reduced at atmospheric pressure and room temperature with H over Pd-C absorbed 1 mole H, the product extracted with ligroine, and distilled gave II. This specimen was identical with the above phenolic product from the reaction of the benzyl ether.

IT **1009-67-2**, Hydrocinnamic acid, α-methyl-
(stereoisomers, and derivs., rearrangement and resolution of)

RN 1009-67-2 HCAPLUS

CN Benzenepropanoic acid, α-methyl- (9CI) (CA INDEX NAME)

CC 10E (Organic Chemistry: Benzene Derivatives)

IT **1009-67-2**, Hydrocinnamic acid, α-methyl-
(stereoisomers, and derivs., rearrangement and resolution of)

L128 ANSWER 53 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN

1959:34688 Document No. 53:34688 Original Reference No. 53:6181c-i,6182a-i,6183a Synthetic studies in the dihydropyrene series. Marvel, C. S.; Wilson, B. D. (Univ. of Illinois, Urbana). Journal of Organic Chemistry, 23, 1483-8 (Unavailable) 1958. CODEN: JOCEAH. ISSN: 0022-3263. OTHER SOURCES: CASREACT 53:34688.

AB A new synthesis of 4,5-dihydropyrene (I) is given. Synthetic expts. designed to produce 1,6-dihydropyrene (II) gave pyrene (III), apparently because of the ease of autoxidation of II. Some expts.

designed to give 1,8-dihydropyrene (IV) are reported, but the synthesis was not completed. I was synthesized by the action of PhLi on 4,5-bis(bromomethyl)phenanthrene (V). An attempted reaction to form I was the cyclodehydration of β-(4-phenanthryl)ethanol (VI) but only a very low mol. weight polymer of 4-vinylphenanthrene was obtained. V (548 mg.) in 50 ml. C6H6 and 200 ml. Et2O treated dropwise during 20 min. with 6 ml. 0.4N PhLi, the mixture stirred 1 hr., refluxed 2 hrs., 150 ml. 0.25% H2SO4 added, the phases separated, the combined organic phases washed with 5% NaHCO3, dried, and distilled gave 278 mg. crude I, m. 132-2.5° (alc.). Chromatography on Al2O3 removed the O containing impurity; picrate, m. 146.5-7.0° (alc.), ν 2835, 2890, 2940, and 3065 cm.-1 (all C-H stretching frequencies), 727, 757, and 831 cm.-1 The ultraviolet spectra was also obtained both in alc. and heptane. VI (1 g.) in 15 ml. concentrated H2SO4 and 5 ml. H2O heated 0.5 hr. on the steam bath, diluted with H2O, and extracted with C6H6 gave an electrostatic powder, in general acting like a low mol. weight polymer, softening at 110° but not fully liquid until 180°. Its average mol. weight was 720. The **infrared** spectrum in Nujol was compatible with a poly(4-vinylphenanthrene) structure, λ 352, 336, 301, and 260 mμ. Attempted cyclization of VI in polyphosphoric acid or by use of anhydrous AlCl3 failed to give any product. 5,8-Bis-(chloromethyl)tetrahydronaphthalene (87.1 g.) in 400 ml. tetrahydrofuran heated to reflux with 3.77 g. LiAlH4 and 11.4 g. LiH with 150 ml. tetrahydrofuran (the addition required 1 hr.), then refluxed a further hr., cooled to 15°, 25 ml. tetrahydrofuran diluted with an equal volume of H2O added dropwise at 15-20°, and then treated with 1 l. 5% H2SO4, extracted with Et2O, washed with dilute acid, H2O, dried, and distilled gave 5,8-dimethyltetrahydronaphthalene (VII), b0.12-0.15 51-4°, n25D 1.5466. VII (32.1 g.) and 3.2 g. Pd-C treated 2 hrs. at 260°, the catalyst removed, and the filtrate distilled gave 28.3 g. 1,4-dimethylnaphthalene (VIII), b0.5-0.7 72-9°, n20D 1.6116. VIII (31.2 g.) in 300 ml. CCl4 refluxed and irradiated 1.5 hrs. with 0.60 g. Bz2O2 and 71.4 g. N-bromosuccinimide, left overnight at room temperature, warmed, filtered hot, the crude residue **digested** with hot CCl4, and crystallized gave 44 g. V, m. 191-1.5°, ν 754, 733, 849, 1450, 1520, and 1591 cm.-1 CH2(CO2Et)2 (500 ml., redistd.) added dropwise to 4 g. Na in 1 l. absolute alc. under reflux, then refluxed 3 hrs., 195 g. V

slurried in 800 ml. C6H6 added over 45 min., the mixture refluxed a further 5 hrs., left overnight at room temperature, hydrolyzed by 500 ml. H2O followed by 500 ml. 20% aqueous HCl, the aqueous phase washed with Et2O, the organic phases washed, and distilled gave 286 g. of residue, crystallized to give 203 g. crude di-Et α,α'-dicarbethoxy-1,4-naphthalenedipropionate (IX), m. 68.5-9.0° (alc.). Saponification and **decarboxylation** of IX gave 97.4% 1,4-naphthalenedipropionic acid (X), m. 257-8°. Ring closure proceeded in liquid anhydrous HF by keeping the temperature low during the mixing. The ring closure was found to proceed best by using small samples of X and by this method 97.0-8.0% yields of crude 2,3-dihydro-1-oxo-1H-phenalene-6-propionic acid (XI), m. 194-8°, were obtained. No attempt was made to purify crude XI. Attempts at ring closure of XI to the dione were unsuccessful in either polyphosphoric acid or H2SO4. Crude XI (4.53 g.) and 90 ml. alc. refluxed 0.5 hr. with 1 ml. concentrated HCl, left 1 hr. at room temperature, concentrated, the residue extracted with hot cyclohexane, the exts. treated with C, and concentrated gave 3.80 g. Et ester (XII) of XI, m. 92-2.5° (cyclohexane). XII (7.98 g.) and 150 ml. 0.5N NaOH refluxed 20 min., cooled to 30°, treated portionwise with 1.50 g. NaBH4, heated 1 hr. at 65°, cooled, dilute HCl carefully added (gas evolution occurred), and the product isolated gave 6.86 g. 2,3-dihydro-1-hydroxy-1H-phenalene-6-propionic acid (XIII), m. 171-3°, ν 3300-200, 2960, 1710, 1604, 1519, 948, 822, 764, and 684 cm.-1 No purification of XIII was attempted. XII (0.5 g.) in 45 ml. alc. treated all at once with 250 mg. NaBH4, stirred at ambient temperature 1 hr., then 1 hr. at 50°, 20 ml. 10% HCl added, extracted with C6H6, washed, and concentrated gave 435 mg. Et ester (XIV) of XIII, m. 110-11° (alc.), ν 3300, 1728, 1603, 1521, 1103, 828, and 769 cm.-1 (Nujol). Attempted cyclization of XIII in liquid anhydrous HF gave a poor yield plus large amts. of carboniferous material. The **infrared** spectrum of this indicated the possible presence of a tetrahydropyrenone. MeMgI (approx. 0.24 mole) treated with 26.9 g. 5-methyl-1-tetrahydronaphthalenone (prepared from o-BrC6H4Me), the crude alc. obtained on hydrolysis and workup of the addition product mixed with 10% of its weight with 10% Pd-C, placed on a bath at 200° and dry N passed over, the temperature raised during 0.5 hr. to

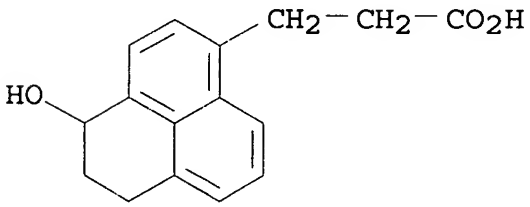
270° (at 210° dehydration began and at 240° dehydrogenation began), the temperature held 1.5 hrs. at 270°, cooled, the product dissolved in C6H6, the catalyst removed, the solvent removed, and distilled gave 23.1 g. 1,5-dimethylnaphthalene (XV), b0.15-0.30, 68-9°, m. 81-2° (MeOH). Bromination of XV as for VIII gave 57.5% 1,5-bis(bromomethyl)naphthalene (XVI), m. 215.5-16.0° (decomposition) (C6H6), ν 695, 789, 1454, 1520, 1599, 2840, and 2920 cm.-1 (Nujol). XVI was converted to 73.1% di-Et α,α'-dicarbethoxy-1,5-naphthalenedipropionate (XVII) by the same procedure used for IX and purified, m. 72.5-3.5° (absolute alc.), ν 1751, 1736, 1599, and 790 cm.-1 (10% in CS2). XVIII (101.9 g.) similarly saponified gave 99.7 g. crude tetracarboxylic acid, dried, and **decarboxylated** by heating 5.5 hrs. at 210°, and the crude product isolated giving 29.6 g. 1,5-naphthalenedipropionic acid (XIX), 302-5° (decomposition). XIX appears to be insol. in all ordinary solvents. XIX in Nujol showed the following bands: ν 2595, 2515, 1707, 1605, 1516, 1301, 948, and 793 cm.-1 XIX (1 g.) refluxed 1.5 hrs. with 20 ml. alc. and 0.60 ml. concentrated HCl gave 0.95 g. di-Et ester, m. 94.5-5.0° (cyclohexane), ν 1737, 1600, 1178, 1165, and 789 cm.-1 (CS2). Similarly, XIX treated with HF gave 87-94% 2,3-dihydro-3-oxo-1H-phenalene-6-propionic acid (XX), m. 148-51°, ν 1729, 1663, 833, and 768 cm.-1 Crude XX esterified as above gave 62% Et ester, m. 46.5-7.0° (cyclohexane-alc.), ν 1739, 1694, 850, and 768 cm.-1 Direct reduction of crude XX was carried out as follows. XX (1 g.) in 50 ml. 0.1N NaOH treated all at once with 500 mg. $NaBH_4$, stirred 0.5 hr. at ambient temperature, then 1 hr. at 50°, reaction ended by addition of 10% HCl, and the product isolated gave 0.84 g. 2,3-dihydro-3-hydroxy-1H-phenalene-6-propionic acid (XXI), m. 114-16° (aqueous MeOH), ν 2680, 2600, 550, 3300, 3160, 1725, 1635, 1604, 1519, 842, and 763 cm.-1 (Nujol). XX Et ester (390 mg.) similarly reduced with $NaBH_4$ gave 122% crude Et ester of XXI and chromatography on Al_2O_3 gave pure product, m. 61-2° (aqueous alc.), ν 3260, 1736, 1603, 1518, 1172, 1104, 839, and 766 cm.-1 Attempts at ring closure of XXI with either liquid anhydrous HF or polyphosphoric acid were unsuccessful. Also, attempted cyclization of the XXI benzoate was unsuccessful with HF. The combined basic insol. material from all the runs of cyclization of XIX, 1.47 g., was extracted with C6H6, concentrated, and precipitated giving 757 mg. 1,2,3,6,7,8-hexahydropyrene-1,6-dione (XXII), plates, m. 239.5-40.5° (C6H6), ν 1675, 1203, 1588, 1519, and 850 cm.-1 (Nujol). XXII was reduced with $NaBH_4$ in alc. but since the solvent was not too good a better method is recommended. Thus 633

mg. XXII, 75 ml. alc., and 0.5 g. NaBH4 stirred 1.5 hrs. at 50°, cooled, treated with 20 ml. 10% HCl, the precipitate collected, and dried gave 516 mg. 1,2,3,6,7,8-hexahydropyrene-1,6-diol (XXIII), m. 240-2°, insol. in most organic solvents, ν 3260, 1673, 1600, 1519, 1304, 1086, 848, and 837 cm.-1 (Nujol). XXIII was somewhat soluble in AcOH and attempted recrystn. gave a product, m. 146-7° (ligroine). The ultraviolet spectrum of this material in alc. indicated 89% III content and the **infrared** spectrum in CS2 was similar to that for III. Chromatography of this material on Al2O3 gave III and a pale yellow band containing insufficient material to permit phys. measurements; the ultraviolet spectrum indicated an oxidation product of III.

IT **6337-29-7**, Phenalene-6-propionic acid, 2,3-dihyro-3-hydroxy-
108836-76-6, Phenalene-6-propionic acid, 2,3(dihydro-3-oxo-
108838-41-1, Phenalene-6-propionic acid, 2,3(dihydro-1-oxo-
118071-16-2, 1,4-Naphthalenedipropionic acid
131459-36-4, Phenalene-6-propionic acid, 2,3-dihyro-1-hydroxy-
(preparation of)

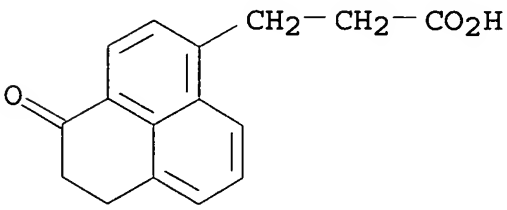
RN 6337-29-7 HCAPLUS

CN Phenalene-6-propionic acid, 2,3-dihydro-3-hydroxy- (6CI, 8CI) (CA INDEX NAME)

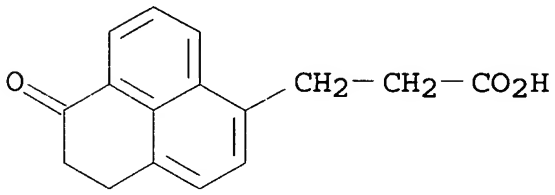


RN 108836-76-6 HCAPLUS

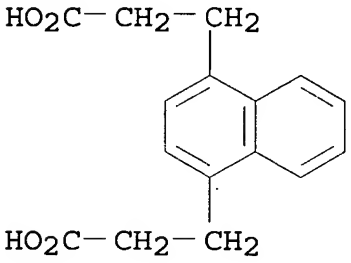
CN Phenalene-6-propionic acid, 2,3-dihydro-3-oxo- (6CI) (CA INDEX NAME)



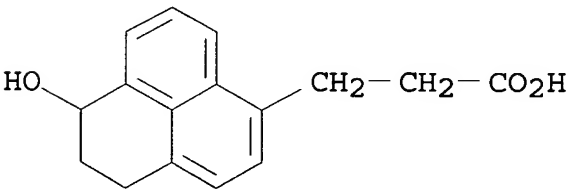
RN 108838-41-1 HCAPLUS
CN Phenalene-6-propionic acid, 2,3-dihydro-1-oxo- (6CI) (CA INDEX NAME)



RN 118071-16-2 HCAPLUS
CN 1,4-Naphthalenedipropanoic acid (9CI) (CA INDEX NAME)



RN 131459-36-4 HCAPLUS
CN Phenalene-6-propionic acid, 2,3-dihydro-1-hydroxy- (6CI) (CA INDEX NAME)



CC 10F (Organic Chemistry: Condensed Carbocyclic Compounds)
IT **Infrared** spectra
Ultraviolet and visible, spectra
(of 4,5-dihydropyrene and related compds.)
IT 571-58-4, Naphthalene, 1,4-dimethyl- 571-61-9, Naphthalene,

1,5-dimethyl- **6337-29-7**, Phenalene-6-propionic acid, 2,3-dihyro-3-hydroxy- 6337-44-6, Malonic acid, [1,4-naphthylenedimethylene]di-, tetraethyl ester 6628-98-4, Pyrene, 4,5-dihydro- 14108-88-4, Naphthalene, 1,2,3,4-tetrahydro-5,8-dimethyl- 21646-18-4, Naphthalene, 1,5-bis(bromomethyl)- 58791-49-4, Naphthalene, 1,4-bis(bromomethyl)- 73562-77-3, Malonic acid, [1,5-naphthylenedimethylene]di-, tetraethyl ester 101168-98-3, 1,6-Pyrenediol, 1,2,3,6,7,8-hexahydro- 101277-98-9, 1,6-Pyrenedione, 2,3,7,8-tetrahydro- 102662-61-3, Pyrene, 4,5-dihydro-, picrate **108836-76-6**, Phenalene-6-propionic acid, 2,3(dihydro-3-oxo- **108838-41-1**, Phenalene-6-propionic acid, 2,3(dihydro-1-oxo- **118071-16-2**, 1,4-Naphthalenedipropionic acid **131459-36-4**, Phenalene-6-propionic acid, 2,3-dihyro-1-hydroxy-
(preparation of)

L128 ANSWER 54 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1958:104054 Document No. 52:104054 Original Reference No. 52:18302d-i
The stereochemistry of ketonization. VI. **Decarboxylation** of 2-phenylcyclohexane-1,1-dicarboxylic acid. Zimmerman, Howard E.; Cutshall, Theodore W. (Northwestern Univ., Evanston, IL). Journal of the American Chemical Society, 80, 2893-6 (Unavailable) 1958. CODEN: JACSAT. ISSN: 0002-7863. OTHER SOURCES: CASREACT 52:104054.
AB cf. C.A. 52, 9970b. PhCH:CHCH:CH2 (64.2 g.) and 85.0 g. CH2:C(CO2Et)2 in 150 cc. C6H6 refluxed 2.5 hrs. and evaporated in vacuo, and the residue recrystd. (hexane) yielded 89.2 g. di-Et ester (I) of 2-phenylcyclohex-3-ene-1,1-dicarboxylic acid (II), m. 77-8°. I (15.7 g.) in 100 cc. EtOAc hydrogenated over 300 mg. PtO2, filtered, and evaporated, and the residue recrystd. (hexane) yielded 8.2 g. di-Et ester (III) of 2-phenylcyclohexane-1,1-dicarboxylic acid (IV), m. 34-6° (hexane). III (10.0 g.) and 11.2 g. KOH in 50 cc. 95% EtOH refluxed 5 hrs., cooled, diluted with 200 cc. H2O, washed with Et2O, acidified with 6N HCl to Congo red, and extracted with Et2O, and the extract worked up yielded 2.10 g. IV, m. 179-80° (EtOAc-ligroine, b. 86-100°). I (54.2 g.) and 78.5 g. KOH in 250 cc. 95% EtOH refluxed 4.5 hrs., cooled, diluted with 500 cc. H2O, washed with Et2O, acidified with 6N HCl, and extracted with Et2O, and the extract worked up gave 26.0 g. acidic material which crystallized (EtOAc-ligroine) yielded 18.3 g. II, m. 185-6°. II (15.0 g.) in 100 cc. EtOAc hydrogenated over 500 mg. PtO2 yielded 10.5 g. IV, m. 177-9° (EtOAc-ligroine). IV (1.00 g.) heated

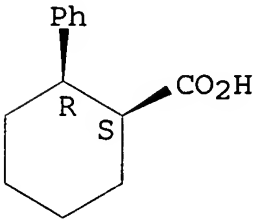
7 min. to 194-9°/1 mm., and the resulting viscous oil (0.81 g.) chromatographed on silica **gel** yielded 0.58 g. cis-2-phenylcyclohexanecarboxylic acid (V), m. 75.0-5.5°, and 0.36 g. trans-V, m. 107.0-8.0°. IV (500 mg.) in 7.5 cc. collidine heated 1 hr. at 60°, cooled, dissolved in 100 cc. Et2O, and extracted with 10% aqueous NaOH, the aqueous extract acidified with 20% HCl to Congo red and extracted with Et2O, the extract subjected to an 8-funnel fractional extraction using in each flask 500 cc. Et2O and 50 cc. pH 7.0 buffer (41.20 cc. 0.2M Na2HPO4 and 8.80 cc. 0.1M citric acid), and each aqueous phase acidified with HCl to Congo red and extracted with Et2O gave in the 1st 2 or 3 funnels the resulting V containing 72.5% cis-V. A series of similar runs was carried out (reaction temperature, reaction time in min., and % cis-V in the product given): 90°, 30, 71.4; 130°, 20, 71.3; 165°, 20, 69.7. IV heated without solvent 8 min. at 195° gave 65.5% cis-V. Pure cis-V (60 mg.) heated 102 hrs. at 200° in a sealed tube gave a mixture of isomers containing 8.5% cis-V; in a run with only 64 hrs. heating time, the product contained 13.7% cis-V. trans-V (60 mg.) heated 102 hrs. at 200° gave a product containing 8.9% cis-V. cis-V (four 60-mg. samples) in 1.0 cc. collidine heated to 60, 90, 110, and 160° for 60, 30, 20, and 20 min., resp., and the mixture analyzed by **infrared** indicated the fractions converted to trans-V to be 0.0472, 0.0298, 0.0396, and 0.0698, resp. The analytical wave lengths for the **infrared** analysis of isomeric V were 7.71 and 7.98 μ.

IT **24905-74-6**, Cyclohexanecarboxylic acid, 2-phenyl-, cis-
24905-75-7, Cyclohexanecarboxylic acid, 2-phenyl-, trans-
(preparation of)

RN 24905-74-6 HCAPLUS

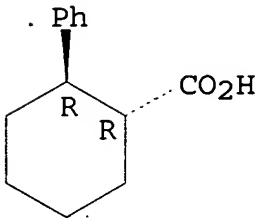
CN Cyclohexanecarboxylic acid, 2-phenyl-, cis- (8CI, 9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 24905-75-7 HCAPLUS
CN Cyclohexanecarboxylic acid, 2-phenyl-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



CC 10E (Organic Chemistry: Benzene Derivatives)
IT **Infrared** spectra
(of cis- and trans-2-phenylcyclohexanecarboxylic acids)
IT **24905-74-6**, Cyclohexanecarboxylic acid, 2-phenyl-, cis-
24905-75-7, Cyclohexanecarboxylic acid, 2-phenyl-, trans-
107620-77-9, 1,1-Cyclohexanedicarboxylic acid, 2-phenyl-
107775-33-7, 3-Cyclohexene-1,1-dicarboxylic acid, 2-phenyl-
109397-17-3, 3-Cyclohexene-1,1-dicarboxylic acid, 2-phenyl-, diethyl ester 109693-04-1, 1,1-Cyclohexanedicarboxylic acid, 2-phenyl-, diethyl ester
(preparation of)

L128 ANSWER 55 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1958:25527 Document No. 52:25527 Original Reference No. 52:4630e-i,4631a-i,4632a-e Structure and properties of certain polycyclic indolo and quinolino derivatives. IX. Derivatives of 1,3,4,5-tetrahydro-5-oxobenz[cd]indole. Mann, Frederick G.; Tetlow, A. J. (Univ. Cambridge, UK). Journal of the Chemical Society, Abstracts 3352-66 (Unavailable) 1957. CODEN: JCSAAZ. ISSN: 0590-9791. OTHER SOURCES: CASREACT 52:25527.
AB 1,3,4,5-Tetrahydro-6-methoxy-1,2-dimethyl-5-oxobenz[cd]indole (I) was prepared by direct cyclization of 3-(2-carboxyethyl)-1,2-dimethyl-5-methylindole (II) followed by remethylation of the intermediate 6-HO derivative (III). The Ph- (IV) and the as-methylphenylhydrazone (V) of I underwent indolization, but the **infrared** evidence indicated that the products, which can be isolated only as salts, were indoline isomers of the expected indolo derivs. I by the Pfitzinger reaction gave 4,6-dihydro-1-methoxy-4,5-dimethylindolo[3,4-bc]acridine-7-carboxylic acid (VI), which formed a colored zwitterion, like previous compds. of this class. When

heated with HCl, VI underwent allylic transformation to the 4,7-dihydro isomer (VII). **Decarboxylation** of VI and VII gave the corresponding isomeric 4,6-dihydro- (VIII) and 4,7-dihydroindoloacridines (IX). These differ from the isomeric pairs of such bases previously described in that they are not interconvertible and they give isomeric instead of identical oxidation products. 1,2-Dimethylindole (X) (5 g.), 3.4 g. CH2:CHCN, 1.7 g. Cu(OAc)2, and 1.7 g. Cu powder heated 12 hrs. at 120-30° in a sealed tube gave 3.5 g. 3-(2-cyanoethyl)-1,2-dimethylindole (XI), m. 108-9° (aqueous alc.). XI was not obtained when the ingredients were heated 15 hrs. at 130-40° with NaOMe, refluxed 6 hrs. in AcOH, or refluxed in dioxane containing benzyltrimethylammonium hydroxide. X (9.2 g.) and 9.2 g. β-propiolactone heated 3 hrs. at 150° gave 7 g. 3-(2-carboxyethyl)-1,2-dimethylindole (XII), m. 153-4° (aqueous alc.). XI hydrolyzed by refluxing with 10% KOH gave XII. XII (3 g.) in 125 cc. Ac2O containing 0.02 g. KCN refluxed 20 hrs., the anhydride removed, and the residue extracted with Et2O gave the anhydride (XIII) of XII, m. 117-18° (alc.). XIII readily hydrolyzed to the free XII. The alc. liquors on evaporation gave a residue which refluxed 15 min. with 5% NaOH gave an oil which gave 1,3,4,5-tetrahydro-1,2-dimethyl-5-oxobenz[cd]indole 2,4-dinitrophenylhydrazone monoethanolate, m. 237-9° (decomposition). The above was typical of numerous attempts to achieve cyclization. The following 3 expts. were directed to the preparation of 1-ethyl-2,5,7-trimethylindole in which the 4-position should have marked activity. 2,4-Me2C6H3NH2 (121 g.) and 109 g. EtBr left 3 days gave the N - Et derivative - H Br, m. 151-2°, which on basification and extraction with Et2O gave N-ethyl-2,4-dimethylaniline (XIV), b0.4 57.5°. XIV (110 cc.), 110 cc. concentrated HCl, and 300 g. ice stirred with cooling while 51.5 g. NaNO2 in 185 cc. H2O was added during 10 min., the stirring continued 1 hr., and the mixture extracted with Et2O gave 112 g. N-ethyl-2,4-dimethyl-N-nitrosoaniline (XV), yellow oil. Attempted reduction of XV with Zn and AcOH gave solely the original aniline. XV (55 g.) in 100 cc. Et2O was slowly added to 12 g. LiAlH4 in 400 cc. Et2O so that gentle refluxing was maintained and after stirring 1 hr. the mixture treated with moist Et2O and then with 75 cc. 30% NaOH giving 35 g. as-ethyl-2,4-dimethylphenylhydrazine (XVI), b0.4 73°. XVI was obtained more satisfactorily by the above method than when conversely the Et2O-LiAlH4 was added to XV. XVI (10 g.) treated with 4.4 cc. Me2CO in AcOH gave 12 g. hydrazone which could not be converted into the indole and its use was abandoned. Me2SO4 (1425

cc.) added to 1845 g. p-MeOC6H4NH2 and heated 2 hrs. at 100° gave crude N-methyl-p-anisidine (XVIa) which dissolved in 2.4 l. concentrated HCl containing 5 kg. ice and treated below 10° with 1.2 kg. NaNO2 in 1.5 l. H2O, and after 1 hr. the product collected, washed, and dried gave 771 g. N-methyl-N-nitroso-p-anisidine (XVII), m. 42-4°. XVII (166 g.) in 320 cc. AcOH added during 3-4 hrs. at 10-20° to 480 g. Zn dust in 600 cc. 50% aqueous alc., after 1 hr. the mixture warmed to 60°, made alkaline with 30% NaOH, and extracted with Et2O gave 3 fractions: (1), 119 g., b. 131-5°; (2), 13 g., b. 137-41°; and (3), 133 g., b. 143-6°. 1 and 2 were XVIa and 3 was N - p - methoxyphenyl - N - methylhydrazine (XVIII). XVIII (152 g.), 80 cc. Me2CO, and 5 cc. AcOH heated 2 hrs., the product added to 1.5 l. alc. saturated with dry HCl, and refluxed 2 hrs. gave 64 g. 5-methoxy-1,2-dimethylindole (XIX), b0.3 134-7°, m. 76.5-7.5° (alc.). In an attempted alternative synthesis, AcCH2Br added to XVIa in alc. containing NaHCO3 at 50° gave p-methoxyphenyl-N-methylaminopropanone, b12 175°, which heated with XVIa and a little HCl gave XIX. XIX (87.5 g.), 36 cc. CH2:CHCN, 30 cc. AcOH, and 5 g. CuCl refluxed 6 hrs. gave 96 g. 3-(2-cyanoethyl)-5-methoxy-1,2-dimethylindole (XX), m. 124.5-5.5° (alc.). XIX (10 g.) and 5 cc. β-propiolactone heated 4 hrs. at 150°, extracted with Et2O, the **polymerized** lactone removed, the Et2O extracted with dilute NaOH, and the Et2O evaporated gave 3.2 g. XIX. Acidification of the alkaline fraction gave 6.7 g. II, m. 119-20.5° (50% aqueous alc.). XX (114 g.) in 500 cc. alc. and 120 g. NaOH in 1.2 l. H2O refluxed 7 hrs. gave 119 g. II. II (20 g.), 100 cc. concentrated H2SO4, and 100 cc. H3PO4 heated 0.5 hr. at 165° gave 4.3 g. III, m. 142-4° (alc.). The aqueous solution extracted with CHCl3 and then with aqueous Na2CO3 and acidified gave 4.3 g. 3-(2-carboxyethyl)-5-hydroxy-1,2-dimethylindole (XXI), m. 147-9° (H2O). XXI cyclized under the same conditions gave III. XXI gave a transient purple color with FeCl3 and with Me2SO4 and aqueous NaOH gave II. XXI was also converted into the 6-p-toluenesulfonyloxy derivative, m. 199-200.5°. III (0.5 g.), 0.5 cc. PhNHNH2, and 0.2 cc. AcOH in 15 cc. alc. refluxed 1 hr. gave 0.66 g. IV, m. 238-9° (C6H6). Similarly prepared were the 6-AcO derivative, m. 157.5-8.5° (alc.); phenylhydrazone of the 6-AcO derivative, m. 224.5-5.5°; 6-p-toluenesulfonyloxy derivative, m. 208-9° (alc.); the corresponding 2,4-dinitrophenylhydrazone, m.

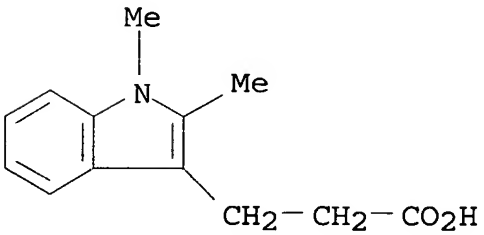
265°; HCl salt, m. 153-4°, very unstable and recrystd. from alc. regenerated the pure indole. III (23.6 g.) in 600 cc. warm Me2CO treated with 10 cc. 30% NaOH and 7 cc. Me2SO4 in alternate addns. until 15 such addns. had been made gave I, m. 144-5° (alc.); the HCl salt was very hygroscopic, gave a satisfactory **infrared** spectrum, and on treatment with 5% NaOH gave I. A warm alc. solution of I when treated with alc.-HCl became deep red but did not deposit crystals, but when taken to dryness and recrystd. from hot Me2CO gave a compound, C14H15O2N.HCl, m. 207° (decomposition), which appeared to be a hydrochloride, but differed from the authentic red salt in that when exposed to air it decomposed much more slowly without becoming sticky, and when treated with 5% NaOH it gave an intractable gum. The nature of this salt was not further investigated. I readily gave IV as plates, m. 150-50.5° (alc.), and V, m. 131-2° (alc.). IV was very stable and was unchanged after 2 years, whereas V had darkened considerably after 4 months. IV (2 g.) in 15 cc. alc. refluxed 3 hrs. with 15 cc. saturated alc. HCl and the mixture left overnight at 0° gave 1 g. 6,11-dihydro-1-methoxy-4,5-dimethyl-4H-indolo[4,3-ab]carbazole-HCl, m. 296° (MeOH); HI salt, m. 304° (decomposition); thiocyanate, needles, m. 279°; picrate, m. 240-1°. Similarly, 1 g. V gave 0.45 g. 6,11-dihydro-1-methoxy-4,5,11-trimethyl-4H-indolo[4,3-ab]carbazole-HCl, m. 343°; hydriodide hemihydrate, m. 341°; perchlorate, m. 314°. I (4.5 g.), 3.3 g. isatin, and 10 cc. 40% KOH refluxed 30 hrs. in 40 cc. alc. gave 5.8 g. VI, red solid, m. 190° (effervescence), soluble in H2O, insol. in CHCl3 and ligroine. When extracted from its solution in AcOH by CHCl3, VI gave the acetate, m. 160-3°, which readily dissociated on recrystn. VI in 10% NaOH gave a yellow solution which deposited crystals of the VI Na salt. VI (1 g.) cautiously heated at 0.001 mm., and the bath temperature finally raised to 300°, melted, effervesced, and gave a sublimate of VIII, m. 156-8°. Carrying out this **decarboxylation** with the initial precipitate, m. 160-3°, a gentle heating at 15 mm. liberating AcOH preceded the stronger heating. This confirmed the identity of the precipitate as an unstable acetate. VIII gave a very hygroscopic red hydrochloride; a red H sulfate, m. 232°; and a maroon hydriodide. VIII in C6H6 exposed 7 days to the air gave a solid residue which could not be crystallized or sublimed in vacuo. VIII in Me2CO oxidized with KMnO4 gave 50% 4,6-dihydro-1-methoxy-4,5-dimethyl-6-oxoindolo[3,4-bc]acridine, m. 220-3° (C6H6); HI salt, m. 296-9° (aqueous alc.); did not form a 2,4-dinitrophenylhydrazone. VI (3.8 g.) in

130 cc. warm H2O treated with concentrated HCl set to a **gel** which on further heating gave a purple solution and after 20 more min. gave 3 g. VII.HCl, m. 160-70°, resolidified, and m. 235° (dilute HCl). VII.HCl (1 g.) heated in a short path sublimation apparatus at 0.001 mm. with the bath temperature rising to 280-300° gave 0.6 g. IX, m. 239-40° (C6H6); maroon HI salt-H2O, m. 310-11° (alc.). Attempts to obtain IX by refluxing solns. in dilute HCl and subsequently basifying failed. There was no evidence that isomerization occurred in these or similar oxidations. IX in C6H6 was unchanged after 5 days exposure to air. IX in Me2CO oxidized with KMnO4 and the residue extracted in a Soxhlet with C6H6 gave 10% 4,7-dihydro-1-methoxy-4,5-dimethyl-7-oxoindolo[3,4-bc]acridine, m. 305-8° (MeOCH2CH2OH)(HI salt-0.5H2O, m. 336-8°), did not form a 2,4-dinitrophenylhydrazone, VI, VII.HCl, VIII, and IX were inactive for antiinflammatory action against egg albumin-induced edema in mice. IX may be slightly active. Ultraviolet absorption spectral curves were given for the above compds.

IT **75535-74-9**, Indole-3-propionic acid, 1,2-dimethyl-
105911-72-6, Indole-3-propionic acid, 5-hydroxy-1,2-dimethyl-
(and derivs.)

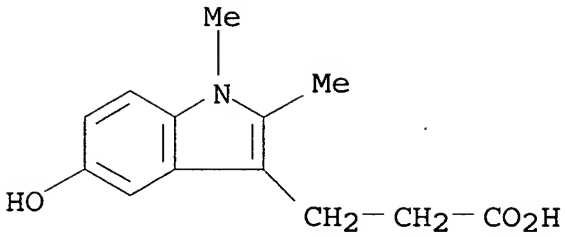
RN 75535-74-9 HCAPLUS

CN 1H-Indole-3-propanoic acid, 1,2-dimethyl- (9CI) (CA INDEX NAME)

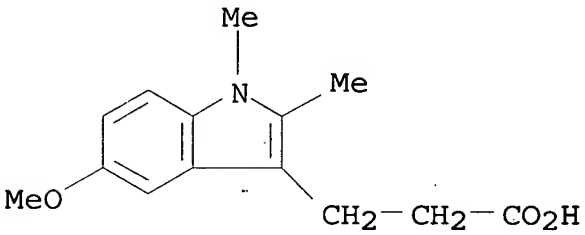


RN 105911-72-6 HCAPLUS

CN Indole-3-propionic acid, 5-hydroxy-1,2-dimethyl- (6CI) (CA INDEX NAME)



IT **106272-76-8**, Indole-3-propionic acid, 5-methoxy-1,2-dimethyl-
(and derivs., and their cyclization)
RN 106272-76-8 HCAPLUS
CN Indole-3-propionic acid, 5-methoxy-1,2-dimethyl- (6CI) (CA INDEX NAME)



CC 10 (Organic Chemistry)
IT **Infrared** spectra
(of benz[cd]indole derivs.)
IT 3744-82-9, Benz[cd]indol-5(1H)-one, 3,4-dihydro- **75535-74-9**, Indole-3-propionic acid, 1,2-dimethyl- **105911-72-6**, Indole-3-propionic acid, 5-hydroxy-1,2-dimethyl- 107662-34-0, Benz[cd]indol-5(1H)-one, 3,4-dihydro-6-hydroxy-1,2-dimethyl- 108874-76-6, Benz[cd]indol-5(1H)-one, 3,4-dihydro-6-methoxy-1,2-dimethyl- 109187-31-7, Benz[cd]indol-5(1H)-one, 3,4-dihydro-1,2-dimethyl- 109647-20-3, 4H-Indolo[4,3-ab]carbazole, 6,11-dihydro-1-methoxy-4,5-dimethyl- 112717-67-6, Indolo[3,4-bc]acridine, 4,6-dihydro-1-methoxy-4,5-dimethyl- 112718-51-1, Indolo[3,4-bc]acridin-7(4H)-one, 1-methoxy-4,5-dimethyl- 112745-04-7, Indolo[3,4-bc]acridine, 4,7-dihydro-1-methoxy-4,5-dimethyl- 115037-23-5, Indolo[3,4-bc]acridine-7-carboxylic acid, 4,7-dihydro-1-methoxy-4,5-dimethyl- 115037-32-6, Indolo[3,4-bc]acridine-7-carboxylic acid, 4,6-dihydro-1-methoxy-4,5-dimethyl-
(and derivs.)

IT **106272-76-8**, Indole-3-propionic acid, 5-methoxy-1,2-dimethyl- (and derivs., and their cyclization)

L128 ANSWER 56 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1957:81412 Document No. 51:81412 Original Reference No. 51:14698f-i,14699a-i,14700a-i,14701a-b Addition of dienophils to azines. Haring, M.; Wagner-Jauregg, T. Helvetica Chimica Acta, 40, 852-71 (Unavailable) 1957. CODEN: HCACAV. ISSN: 0018-019X.

AB The addition of (PhCH: N)2 (I) to dienophils other than maleic anhydride (II), and the reaction of dienophils with various azines were investigated (cf. Kov.acte.acs, et al., C.A. 46, 2521a, 8649e). I (50 g. dried in high vacuum), 55 g. II, and 50 ml. absolute xylene heated 20 hrs. at 145-50°, the resinous product **digested** with AcOH, and the powdery residue washed with AcOH and Et2O gave 36 g. 1,5-disubstituted pyrazolidino-[1,2]pyrazolidine-2,3,6,7-tetracarboxylic anhydride (III) [substituents = Ph (IV)], m. 248-9°. I (461 g.) and 900 ml. H2C:CHCO2Me (V) autoclaved 2 days at 125-30°, the oily product taken up in 1:1 Me2CO-MeOH and treated with 350 mg. picric acid in Me2CO, filtered after several hrs. and the residue washed thoroughly gave 305 g. crude picrate, m. 207° (from Me2CO). The picrate suspended in 8 l. H2O and treated with 80 g. dry Na2CO3, the free base extracted with 1 l. C6H6, the dried extract evaporated and the residue stirred with cold petr. ether, filtered, and the precipitate washed with petr. ether gave 175.7 g. mixture of stereoisomers of di-Me 1,5-diphenylpyrazolidino[1,2]pyrazolidine-2,6-dicarboxylate (VI), m. 137° (from C6H6-petr. ether and dilute MeOH); methiodide, m. 202°; ethobromide, m. 199°; dihydrazide, m. 217-21° (decomposition). VI (5 g.) heated 18 hrs. in a sealed tube with 8.2 g. Et2NCH2CH2NH2 at 90°, the cooled product poured into H2O, filtered and the filtrate percolated 3 days with C6H6, the extract evaporated, the residue dried on a porous plate, and crystallized from ligroine gave 0.56 g. VI bis(diethylaminoethylamide) (VII), m. 169-71°. VI (10 g.) extracted in a Soxhlet apparatus with 200 ml. absolute Et2O over 4 g. LiAlH4, the product carefully decomposed with H2O with external cooling, filtered, the slimy residue extracted with boiling alc., and the extract evaporated yielded 7.8 g. crystalline 1,5-diphenyl-2,6-bis(hydroxymethyl)pyrazolidin

o[1,2]pyrazolidine (VIII), m. 199° (from dilute alc.), soluble in dilute acids. VI (10 g.) distilled at 200-20°/10 mm. gave V (decolorizing 5% Br in CCl4) and 7.9 g. viscous oily product. The oil taken up in Et2O, the solution extracted 3 times with N HCl (yielding 0.4 g. VI) and 3 times with 1:1 aqueous HCl, the extract evaporated and the yellow oil (3.2 g.) distilled at 130°/0.002 mm., the distillate taken up in Et2O and diluted with petr. ether, and the mixture refrigerated gave Me 1-benzyl-3-phenyl-2-pyrazoline-4-carboxylate, m. 62.5-3.0°, saponified to the corresponding acid, m. 108°, **decarboxylated** by heating at 80-90°/10 mm. and distillation at 130°/0.001 mm. to 1-benzyl-3-phenyl-2-pyrazoline (IX), m. 94-5°. The original Et2O extract (after removal of basic constituents) evaporated and the residue (2.1 g.) distilled at 127-30°/10 mm. gave PhCH:CHCO2Me, m. 35-6°, [α]D20 1.5710; saponified to PhCH:CHCO2H, m. 132-3° (from C6H6-petr. ether). VI (175.5 g.) refluxed 15 hrs. with 54.6 g. KOH in 350 ml. absolute alc., the solution evaporated in vacuo, the residue taken up in 500 cc. H2O and filtered, the filtrate stirred with 78.7 ml. concentrated HCl, filtered, the residue taken up in NaOH, precipitated with HCl, and the product dried at 110°/0.001 mm. gave 1,5-diphenylpyrazolidino[1,2]pyrazolidine-2,6-dicarboxylic acid (X). X (5 g.) **decarboxylated** 10 min. at 270-5°, the melt **digested** with Et2O and the Et2O extract washed with 80 ml. 5% aqueous NaHCO3, the aqueous phase acidified with concentrated HCl and refrigerated, filtered, the residue (0.45 g., m. 117-20°) sublimed at 100°/0.001 mm., and the sublimate crystallized from C6H6-petr. ether gave PhCH:CHCO2H, m. 132.5-3.0°. The Et2O extract (freed from PhCH:CHCO2H) extracted with N HCl and again with 1:1 aqueous HCl yielded 0.5 g. 2-methyl-3-phenyl-4-pyrazoline, b0.01 60°, nD20 1.5958, and 0.5 g. IX. IX (0.5 g.) stirred 3 hrs. at 15-25° in 100 ml. Me2CO with addition of 4 g. KMnO4, the mixture diluted with 50 ml. H2O and the Me2CO evaporated at 40° in vacuo, filtered, and the filtrate acidified with concentrated HCl gave 0.1 g. BzOH, m. 121°. The precipitate extracted with Et2O, the extract evaporated, the residue distilled at 120°/0.01 mm., and the crystalline fraction recrystd. from petr. ether gave 0.2 g. 1-benzyl-3-phenylpyrazole, m. 58-60°; picrate, m. 113-14°. X (20 g.) in 500 ml. H2O containing 4.8 g. NaOH treated in 5 hrs. by dropwise addition of 46 g.

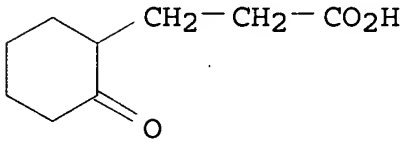
KMnO4 in 2 l. H2O at 0-3°, the mixture kept 15 hrs. at room temperature and cleared with addition of 16 g. NaHSO3, filtered and the filtrate concentrated in vacuo, the concentrate extracted 3 times with Et2O, the extract evaporated, and the product crystallized from ligroine-C6H6 gave the known 3-phenylpyrazole, m. 76-8°; picrate, m. 171-2°. The original aqueous solution acidified with 34 ml. concentrated HCl and extracted with Et2O, filtered [the residue crystallized from AcOH with addition of H2O and Et2O yielded 7.0 g. colorless unknown substance, C20H18N2O6, m. 238-40° (gas evolution)] and the filtrate evaporated, the residue sublimed, and the sublimate crystallized from H2O gave 2.0 g. BzOH, m. 121°. The aqueous phase extracted 15 hrs. with Et2O, the product taken up in a little cold H2O, filtered, and the filtrate slowly evaporated by exposure on a clock-glass gave (CO2H)2.2H2O, m. 95°. Based on the above degradation reactions the criss-cross addition of I [and 2-furalazine (XI)] and H2C:CHCO2R produces a bis(pyrazolidine) ring system whose constitution is conformed by the close similarity of the **infrared** spectra of IV and the corresponding tetramethyl ester and comparison with the related parent 1,5-diphenylpyrazolidino[1,2]pyrazolidine. XI (49.5 g.), 120 ml. V, and 1 g. hydroquinone autoclaved 18 hrs. at 138-42°, the oily product taken up in 250 ml. Me2CO and warmed with 50 g. picric acid, the mixture cooled to 0°, filtered, and the precipitate washed gave 20 g. picrate, m. 196-7°, converted to 10.1 g. di-Me 1,5-di(α-furyl)pyrazolidino[1,2]pyrazolidine-2,6-dicarboxylate, m. 106° (from C6H6-petr. ether); dihydrazide, m. 229-30° (from H2O). I (5 g.) and 3 g. H2C:CHCN heated 36 hrs. at 135-42° in a steel tube, the product taken up in Me2CO, precipitated with Et2O, and the product (0.15 g., m. 218°) crystallized from C6H6-Et2O or AcOH gave difficultly reproducible 2,6-dicyano-1,5-diphenylpyrazolidino[1,2]pyrazolidine, m. 223-4°. (MeCH:CHCH:N)2 [cf. Hl.acte.adik, Monatsh. 24, 438(1903)] (15 g.) and 50 ml. V heated 2 days in the presence of a trace of hydroquinone at 140° in a steel tube, the excess ester distilled, and the residue fractionated gave a liquid base, C16H24N2O4, b3 115-23°, nD20 1.4917, for which alternative bis(pyrazolidine) and bipyridyl structures are proposed. (EtCH:N)2 (200 ml.), 400 ml. V, 400 ml. absolute xylene, and 0.5 g. hydroquinone refluxed 4 days, excess solvent and material distilled at 15 mm., and

the residue fractionated through a 15 cm. Raschig-ring column gave 10.7 g. fraction 1, b1.0 77-83°, nD20 1.4652 g. (methiodide, C11H21IN2O2), 41.4 g. fraction 2, b1.0 93-5°, nD20 1.4668, and 1.0 g. fraction 3, b3 170-6°, nD20 1.4720. Cyclohexanone azine (40 g.) and 55 cc. (:CHCO2Me)2 refluxed 24 hrs. and the product distilled in high vacuum, the oily product (b0.04 138-47°) kept 1-2 weeks and triturated with C6H6-petr. ether, filtered, and the washed powder crystallized from ligroine and C6H6-petr. ether gave 5 g. compound, C26H38N4O7, converted by boiling 2 hrs. in H2O to a crystalline compound, C22H30N2O6, m. 170° (from C6H6), containing no CO2H or CO groups and not cleaved by concentrated HCl to give N2H4. Cyclohexanone azine (40 g.), 80 ml. V, and 0.5 g. hydroquinone heated 24 hrs. in a steel tube at 145°, the mixture distilled in high vacuum, and the residue fractionated gave a substance, C18H26N2O2, b0.01 90-140°, m. 149-50° (from C6H6-petr. ether), an oily intermediate fraction, and 13.6 g. di-Me bis(cyclohexanone-2-propionate) azine, b0.01 170-90°, nD20 1.5100. The azine (5 g.) in 10 ml. MeOH kept 30 min. at room temperature with 3 ml. concentrated HCl, filtered from 0.65 g. precipitated N2H4.HCl, the filtrate evaporated, taken up in aqueous NaHCO3 and extracted with Et2O, the dried extract evaporated, and the residue distilled in vacuo gave Me cyclohexanone-2-propionate, b11 135-7°, nD20 1.4640, saponified to the free acid, m. 64-6°. A mechanism for the unexpected 1,2-addition with formation of the azine is postulated. XI (45 g.), 75 g. II, and 150 ml. C6H6 refluxed 18 hrs., the mixture cooled and diluted with Me2CO to dissolve the resinous byproduct, filtered, and the crystalline condensation product (20 g.) recrystd. from Ac2O-C6H6 gave 1,5-di(α-furyl) substituted III (XII), m. 224°. XII (2.0 g.) in 20.8 ml. N NaOH filtered and the filtrate treated with 21.0 ml. N HCl, filtered immediately and the filtrate kept 2 days, filtered, and the crystalline precipitate dried at 0.001 mm. gave 1.3 g. corresponding tetracarboxylic acid (XIII), m. 219°. Analogou s condensations of substituted benzalazines with II gave III (1 and 5 substituent, % yield, m.p. given): p-ClC6H4 (XIV), 20, 284°; p-AcOC6H4 (XV), 48, 258-60°; p-MeOC6H4 (XVI), 60, 270-1°; p-Me2NC6H4 (XVII), 80, 281.5-2.5°; o-O2NC6H4 (XVIII), 49, 272°. XIV gave the corresponding

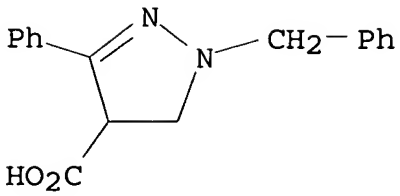
tetracarboxylic acid, m. 253°. XV (3 g.) refluxed 15 hrs. with 26 g. 20% aqueous KOH, the solution diluted with H2O and treated with 17 cc. concentrated HCl (d. 1.19), the mixture evaporated and the residue taken up in a min. of H2O, kept several days at 0°, and filtered gave 1.1 g. 1,5-bis(p-hydroxyphenyl)pyrazolidino[1,2]pyrazolidine-2,3,6,7-tetra-carboxylic acid, m. 227°. XVI was converted as above to the corresponding tetracarboxylic acid (XIX), m. 231.5°. XVI (15 g.) and 7.5 g. Et2NCH2CH2NH2 heated 30 min. at 195° at atmospheric pressure and 5 min. at 14 mm., the cooled product taken up in cold HCl, filtered, the filtrate neutralized with N NaOH and the product crystallized from ligroine-C6H6 gave 4.2 g. colorless XVI bis(diethylaminoethylimide), m. 215-16°. XVI (5 g.) added with vigorous stirring at 20° to 100 ml. dioxane, 10 g. HONH2.HCl, and 10 g. anhydrous NaOAc, the mixture stirred 15 min. and refluxed 1 hr., the cooled mixture filtered and the precipitate washed with dioxane and H2O, the colorless powder taken up in 5% NaHCO3 solution and filtered, the filtrate acidified with concentrated HCl, and the product dried at 110°/3 mm. gave XVI bis(N-hydroxyimide), m. 312-14°, no color with FeCl3. XVII (30 g.) in 150 ml. absolute xylene at 100° treated dropwise in 15 min. with 18 ml. Et2NCH2CH2NH2 in 50 ml. absolute xylene, the mixture distilled to give 185 ml. distillate, diluted with 250 ml. xylene and distilled to give 50-70 ml. distillate, the combined distillate boiled with C and filtered through a steam-funnel, the filtrate diluted with ligroine, filtered, and the residue crystallized from C6H6MeOH gave 3.5 g. colorless XVII bis(diethylaminoethylamide), m. 246-8°. XVIII (10.5 g.) in 85 ml. N NaOH, the solution diluted with 100 ml. H2O and hydrogenated in the presence of 0.1 g. PdO, the mixture filtered, the filtrate treated with 84 ml. N HCl, filtered, and the product dried at 100°/3 mm. gave 1,5-bis(o-aminophenyl)pyrazolidino[1,2]pyrazolidine-2,3,6,7-tetracarboxylic acid, m. above 320°, insol. in organic solvents, soluble in N acids and bases. The HN:CO-I addition compound, 3,7-dioxo-1,5-diphenyl-s-triazolidino[a]-s-triazolidine (cf. Bailey and Moore, C.A. 11, 589)(10.1 g.) extracted in a Soxhlet apparatus with 300 ml. dioxane over 5 g. LiAlH4, the product carefully decomposed with AcOH and H2O (smell of NH3), filtered and the residue extracted with boiling dioxane, the combined filtrates evaporated in vacuo, the

partially crystalline residue (4.6 g.) dried on a porous plate, and the powdery product (0.7 g.) crystallized from alc. gave 5-hydroxy-3-phenyl-1,2,4-triazolidine (XX), m. 159.5°. The porous plate extracted exhaustively with boiling Et2O, the extract evaporated, and the residue fractionated gave PhCH2NHMe, b38 96.0-7.5°, nD20 1.5235. The toxicity and pharmacol. activity of the addition products of alazines with II or V was, in general, very small but the introduction of basic substituents increased greatly the pharmacol. activity of individual compds. Thus, VII given intravenously had LD50 15 mg./kg. in the mouse. In rabbits, VI had less antipyretic activity than aminopyrine. In the mouse per os 100 mg. XIX/kg. had no antipyretic but a very slight analgesic effect, and 500 mg. XX/kg. had strong sedative but insignificant analgesic actvity. No antipyretic effects were produced by these compds. in guinea pigs. In the rat, intravenous administration of 50-100 mg. XIII Na salt/kg. or 5 mg. VII/kg. definitely raised, whereas 20 mg. VIII/kg. briefly lowered the blood pressure.

IT **2275-26-5**, Cyclohexanepropionic acid, 2-oxo-
(and derivs.)
RN 2275-26-5 HCAPLUS
CN Cyclohexanepropanoic acid, 2-oxo- (9CI) (CA INDEX NAME)



IT **102025-68-3**, 2-Pyrazoline-4-carboxylic acid, 1-benzyl-3-phenyl-(?)
(preparation of)
RN 102025-68-3 HCAPLUS
CN 2-Pyrazoline-4-carboxylic acid, 1-benzyl-3-phenyl- (6CI) (CA INDEX NAME)



CC 10 (Organic Chemistry)

IT **2275-26-5**, Cyclohexanepropionic acid, 2-oxo- 112349-80-1, 1H,5H-Pyrazolo[1,2-a]pyrazole-2,6-dicarboxylic acid, tetrahydro-1,5-diphenyl-
(and derivs.)

IT 729-19-1, 2-Pyrazoline, 1-benzyl-3-phenyl-(?) 2458-26-6, Pyrazole, 3(or 5)-phenyl- 5396-52-1, 1H,5H-Pyrazolo[1,2-a]pyrazole-1,2,5,6-tetracarboxylic 1,2:5,6-dianhydride, tetrahydro-3,7-diphenyl- 6456-07-1, Pyrazole, 3(or 5)-phenyl-, picrate 7188-90-1, Pyrazole, 1-benzyl-3-phenyl- 18076-03-4, 2-Pyrazoline, 1-methyl-3-phenyl-(?) 98594-27-5, 1,2,4-Triazolidin-3-ol, 5-phenyl- 101793-19-5, 2-Pyrazoline-4-carboxylic acid, 1-benzyl-3-phenyl-(?), methyl ester **102025-68-3**, 2-Pyrazoline-4-carboxylic acid, 1-benzyl-3-phenyl-(?) 102452-79-9, Pyrazole, 1-benzyl-3-phenyl-, picrate 108726-07-4, 1H,5H-Pyrazolo[1,2-a]pyrazole, tetrahydro-1,5-dipropenyl-(?) 109594-20-9, 1H,5H-Pyrazolo[1,2-a]pyrazole-1,2,5,6-tetracarboxylic 1,2:5,6-dianhydride, 3,7-di-2-furyltetrahydro- 109964-76-3, 1H,5H-Pyrazolo[1,2-a]pyrazole-1,2,5,6-tetracarboxylic acid, 3,7-di-2-furyltetrahydro- 113062-07-0, 1H,5H-Pyrazolo[1,2-a]pyrazole-2,6-dicarbonitrile, tetrahydro-1,5-diphenyl- 114306-56-8, 1H,5H-Pyrazolo[1,2-a]pyrazole-2,6-dimethanol, tetrahydro-1,5-diphenyl- 115048-44-7, 1H,5H-Pyrazolo[1,2-a]pyrazole-1,2,5,6-tetracarboxylic acid, tetrahydro-3,7-bis(p-hydroxyphenyl)- 115052-24-9, 1H,5H-Pyrazolo[1,2-a]pyrazole-1,2,5,6-tetracarboxylic acid, 3,7-bis(p-chlorophenyl)tetrahydro- 115164-91-5, 1H,5H-Pyrazolo[1,2-a]pyrazole-1,2,5,6-tetracarboxylic 1,2:5,6-dianhydride, 3,7-bis(p-chlorophenyl)tetrahydro- 115164-92-6, 1H,5H-Pyrazolo[1,2-a]pyrazole-1,2,5,6-tetracarboxylic 1,2:5,6-dianhydride, tetrahydro-3,7-bis(o-nitrophenyl)- 118951-31-8, 1H,5H-Pyrazolo[1,2-a]pyrazole-1,2,5,6-tetracarboxylic 1,2:5,6-dianhydride, tetrahydro-3,7-bis(p-methoxyphenyl)- 119248-58-7, 1H,5H-Pyrazolo[1,2-a]pyrazole-1,2,5,6-tetracarboxylic 1,2:5,6-diimide, N,N'-bis(2-diethylaminoethyl)-3,7-bis(p-dimethylaminophenyl)tetrahydro- 121235-02-7, 1H,5H-Pyrazolo[1,2-a]pyrazole-1,2,5,6-tetracarboxylic 1,2:5,6-diimide,

N,N'-bis(2-diethylaminoethyl)tetrahydro-3,7-bis(p-methoxyphenyl)- 121760-78-9, 1H,5H-Pyrazolo[1,2-a]pyrazole-1,2,5,6-tetracarboxylic 1,2:5,6-dianhydride, 3,7-bis(p-dimethylaminophenyl)tetrahydro- 121969-57-1, 1H,5H-Pyrazolo[1,2-a]pyrazole-2,6-dicarboxamide, N,N'-bis(2-diethylaminoethyl)tetrahydro-1,5-diphenyl- 122725-01-3, 1H,5H-Pyrazolo[1,2-a]pyrazole-1,2,5,6-tetracarboxylic 1,2:5,6-diimide, tetrahydro-N,N'-dihydroxy-3,7-bis(p-methoxyphenyl)- 122725-05-7, 1H,5H-Pyrazolo[1,2-a]pyrazole-1,2,5,6-tetracarboxylic acid, tetrahydro-3,7-bis(p-methoxyphenyl)- 122767-11-7, 1H,5H-Pyrazolo[1,2-a]pyrazole-1,2,5,6-tetracarboxylic 1,2:5,6-dianhydride, tetrahydro-3,7-bis(p-hydroxyphenyl)-, diacetate 124144-65-6, 1H,5H-Pyrazolo[1,2-a]pyrazole-1,2,5,6-tetracarboxylic acid, 3,7-bis(o-aminophenyl)tetrahydro- 856796-91-3, 1,1'(2H,2'H)-Binicotinic acid, 3,3',4,4'-tetrahydro-4,4'-dimethyl-, dimethyl ester
(preparation of)

L128 ANSWER 57 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1957:25460 Document No. 51:25460 Original Reference No. 51:5039b-f
Synthesis and **polymerization** of vinyl derivatives of furan and thiophene. Andreeva, I. V.; Koton, M. M. (Inst. High Polymers, Acad. Sci. U.S.S.R., Moscow). Doklady Akademii Nauk SSSR, 110, 75-8 (Unavailable) 1956. CODEN: DANKAS. ISSN: 0002-3264.

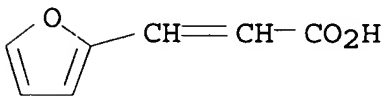
AB 2-Vinylfuran (by **decarboxylation** of furylacrylic acid), b764 96-7°, nD28 1.4994; 2-vinylthiophene (from thienylmagnesium iodide and ethylene oxide, the alc. **dehydrated** with solid KOH), b48 66.5°, nD20 1.5722. The following vinyl derivs. were prepared by Meerwein-Ponndorf reduction of corresponding ketones, the alcs. being **dehydrated** over Al2O3. Me benzofuryl ketone was prepared by ring closure condensation of salicylaldehyde and MeCOCH2Cl. The following vinyl derivs. were used for **polymerization** studies: 2-vinylbenzofuran, b0.16 52°, nD25 1.6020; 2-vinyldibenzofuran, b0.5 130°, b2 147°, m. 31°, nD30 1.6572; 2-vinyldibenzothiophene, b0.05 167°, m. 42°. Kinetics of **polymerization** of the above were shown by reaction curves obtained dilatometrically with 0.5% Bz2O2 as catalyst at 60°, 80°, 90° and 100°; LiBu at 35°, and BF3-Et2O at 0° were also examined as catalysts. Since O affected the **polymerization** rates in these cases, atmospheric O was rigidly excluded. From the **polymerization** rates at the indicated temps. the activation energy for peroxide catalysis was found to be: 2-vinylfuran 17, cal./mole; 2-vinylbenzofuran, 16.5; 2-vinyldibenzofuran, 12.4. The rate of **polymerization** increased with increased number of

condensed rings on furan for both radical and ionic processes. Activation energy for **polymerization** of 2-vinylthiophene in the peroxide catalyzed reaction was 16 cal./mole. Vinyldibenzothiophene **polymerized** much more rapidly than did vinylthiophene. With radical catalysts a stepwise elevation of temperature during the reaction yielded polymers with almost unchanged properties over the conventional constant temperature products. Vinyldibenzofuran polymers showed higher viscosity, and hence mol. weight, than those from vinylbenzofuran. The high mol. weight products had dielectric properties identical with those of the low mol. weight products. The m.ps. tended to decline with increase of the number of condensed rings in a given monomer, S-derivs. being lower melting than O-derivs.

IT **539-47-9**, 2-Furanacrylic acid
(carboxyl-group removal from)

RN 539-47-9 HCAPLUS

CN 2-Propenoic acid, 3-(2-furanyl)- (9CI) (CA INDEX NAME)



CC 10 (Organic Chemistry)

IT Activation energy
(Heat of activation, of **polymerization**, of vinyl compds.)

IT Catalysts
(in **polymerization**, of vinyl compds.)

IT Reaction kinetics and(or) velocity
(of **polymerization**, of vinyl derivs. of furan and thiophene)

IT **Polymerization**
(of vinyl derivs. of furan and thiophene)

IT 1487-18-9, Furan, 2-vinyl- 1918-82-7, Thiophene, 2-vinyl-
(and derivs., **polymerization** of)

IT 109-72-8, Lithium, butyl-
(as catalyst in **polymerization** of vinyl compds.)

IT 94-36-0, Benzoyl peroxide
(as catalyst in **polymerization**, of vinyl compds.)

IT **539-47-9**, 2-Furanacrylic acid
(carboxyl-group removal from)

IT 7637-07-2, Boron fluoride

(catalysts from Et2O and, in **polymerization** of vinyl compds.)
IT 7782-44-7, Oxygen
(in **polymerization**, of vinyl compds., reaction kinetics and)
IT 110-00-9, Furan 110-02-1, Thiophene
(vinyl derivs., **polymerization** of)

L128 ANSWER 58 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1955:69021 Document No. 49:69021 Original Reference No. 49:13198e-i,13199a-i,13200a-b The preparation of polycyclic aromatic hydrocarbons from arylpropiolic acids. Campbell, A. D. (Univ. Glasgow, UK). Journal of the Chemical Society, Abstracts 3659-69 (Unavailable) 1954. CODEN: JCSAAZ. ISSN: 0590-9791. OTHER SOURCES: CASREACT 49:69021.
GI For diagram(s), see printed CA Issue.
AB cf. Wojack, et al. C.A. 32, 7442.7. 2,3-Benzoperylene (I), naphtho-2',3',1,2-pyrene (II), 1,2:3,4:5,5a,6:11,11a,12-tetrabenzonaphthacene (III), and 1,2-benzopyrene (IV) have been synthesized by **decarboxylation** and cyclodehydrogenation of the products of dimerization of a series of arylpropiolic acids. Several fluorenones have been prepared by **decarboxylation** of the acids obtained by intramol. cyclization of the dimerization products. PhC.tplbond.CCO2H (V), 2-C10H7C.tplbond.CCO2H (VI), and 9-phenanthrenepropiolic acid (VII) were prepared by bromination, followed by dehydrobromination of the corresponding acrylic acids. Bromination of 5,6,7,8-tetrahydro-2-naphthaleneacrylic acid in CCl4 or with pyridine-HBr perbromide gave, with the evolution of HBr, in the latter case a crystalline di-Br acid where H had been replaced. The required tetrahydronaphthalenepropiolic acid was synthesized by carboxylation of the Grignard derivative of 6-ethynyl-1,2,3,4-tetrahydronaphthalene, prepared from 6-acetyl-1,2,3,4-tetrahydronaphthalene by treatment with PCl5 followed by dehydrohalogenation. Refluxing 1-C10H7C.tplbond.CO2H with Ac2O gave the dimer, 1-(1-naphthyl)-2,3-phenanthrenedicarboxylic anhydride (VIII), m. 232°. The insol. K salt derived therefrom was **decarboxylated** when heated with soda-lime and Cu powder in vacuo, to a mixture of I, formed by simultaneous dehydrogenation, and 1-(1-naphthyl phenanthrene, m. 115°. These products were not readily separated by chromatog., but were separated by means of their 1,3,5-C6H3(NO2)3 complexes. The 2 hydrocarbons were also obtained, but in lower yield, by direct distillation of the dry Na salt formed from the anhydride. No cyclization took place on treatment of VIII with

anhydrous HF although the isomeric naphthyl-2,3-phenanthrenedicarboxylic anhydride (IX) gave a fluorenone under similar conditions. Cyclization of VIII with AlCl3 in PhNO2 gave a good yield of the very soluble 9-oxo-5,6-benzonaphtho-1',2',3,4-fluorene-1-carboxylic acid (X), m. 294-6°, which was readily **decarboxylated** to the brick red 5,6-benzonaphtho-1',2',3,4-fluorenone (XI). The carbonyl ring of XI was opened by fusion with KOH to give a carboxylic acid which was **decarboxylated** to 1-(1-naphthyl)phenanthrene. Dimerization of VI with Ac2O gave excellent yields of IX. Chromatog. separation of the products obtained by direct **decarboxylation** of this anhydride by sublimation from Cu-bronze and soda-lime in vacuo gave 4-(2-naphthyl)phenanthrene, together with 2 isomeric ketones which are probably 7,8- (XII) and 6,7-benzonaphtho-2',1',3,4-fluorenone (XIII). Both XII and XIII gave K salts when fused with KOH, and the acids obtained from them were **decarboxylated** to 4-(2-naphthyl)phenanthrene, showing that the ketones differ only in the point of attachment of the carbonyl group in the naphthalene nucleus. Further, both K salts sublimed from Cu-bronze, gave II, m. 258-9°. Intramol. cyclization of 4-(2-naphthyl)-2,3-phenanthrenedicarboxylic anhydride with AlCl3 in PhNO2 or with anhydrous HF gave the same keto acid. On the assumption that normal cyclization took place with the new ring attached to the 1- rather than to the 2-position of the naphthalene nucleus, this compound was given the structure of 9-oxo-7,8-benzonaphtho-2',1',3,4-fluorene-1-carboxylic acid (XIV). **Decarboxylation** with Cu-bronze in quinoline then gave the red V, m. 239°. The 2 isomeric fluorenones were readily reduced by N2H4.H2O in good yield to 7,8- and 6,7-benzonaphtho-2',1',3,4-fluorene, which had similar UV absorption spectra. Reduction of 7,8-benzonaphtho-2',1',3,4-fluorenone with Zn dust in AcOH gave the corresponding fluorenol which on distillation from Zn dust yielded 7,8-benzonaphtho-2',1',3,4-fluorene, identical with that obtained by reducing the fluorenone with N2H4.H2O. Cyclodehydrogenation of 4-(2-naphthyl)phenanthrene with AlCl3-NaCl at 140° gave only **polymerized** material, but at temps. below 120° II was obtained. 1-(9-Phenanthryl)-2,3-triphenylenedicarboxylic anhydride (XV), obtained by dimerizing VII, was **decarboxylated** by heating the dry Na salt of the acid in vacuo with powdered soda-lime and Cu powder to a pale yellow sublimate which was chromatographed on alumina, the product being 1-(9-phenanthryl)triphenylene (XVI), and III, the latter being formed by simultaneous **decarboxylation** and cyclodehydrogenation. XVI, which formed a mol. complex with 2 mols.

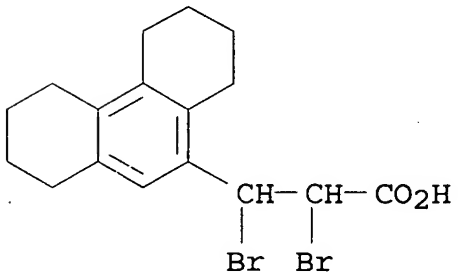
of 1,3,5-C6H3(NO2)3, gave III on cyclodehydrogenation with Pd-C. In all the above reactions dimerization was between identical mols. However, when V and IV reacted a mixture of 3 of the 4 possible combinations was isolated but complete separation proved very tedious: 4-phenyl-3,4-phenanthrenedicarboxylic anhydride (XVI), flat needles, m. 233°, formed by a mixed combination, was isolated together, with 1-phenyl-2,3-naphthalenedicarboxylic anhydride, m. 252° and 4-(2-naphthyl)-2,3-phenanthrenedicarboxylic anhydride, m. 265°. PhC.tplbond.CCOCl and VI in C6H6 gave XVI and 1-(2-naphthyl)-2,3-naphthalenedicarboxylic anhydride (XVII), the latter characterized by **decarboxylation** to 1,2'-binaphthyl, orange needles, m. 123-4°. On further cyclization with anhydrous AlCl3 in PhNO2 XVII gave 9-oxo-3,4:7,8-dibenzofluorene-1-carboxylic acid, which was **decarboxylated** with Cu-bronze to 1,2:5,6-dibenzofluorenone. **Decarboxylation** of 4-phenyl-2,3-phenanthrenedicarboxylic anhydride (XVIII) by subliming the derived K salt from soda-lime and Cu powder, gave a low yield of 4-phenylphenanthrene (XIX), m. 80-1°, and also 1,2-benzopyrene, pale yellow plates, m. 175°, formed by simultaneous cyclodehydrogenation. XVIII failed to give derivs. with picric acid and 1,3,5-C6H3(NO2)3, but it had identical properties with a sample prepared by **dehydration** and dehydrogenation of the product obtained by treating PhLi with 1,2,3,4-tetrahydro-4-oxophenanthrene. The absorption spectrum of XIX showed predominately the phenanthrene structure and resembled closely that of 4-(2-naphthyl)phenanthrene. Cyclization of XVIII gave 9-oxonaphtho-2',1',3,4-fluorene-1-carboxylic acid, m. 240°, **decarboxylated** to naphtho-2',1',3,4-fluorenone, orange needles, m. 148-9°. Dimerization of 5,6,7,8-tetrahydro-2-naphthylalenepropiolic acid with Ac2O gave a mixture of 2 isomeric anhydrides. Fractional crystallization gave 5,6,7,8-tetrahydro-4-(5,6,7,8-tetrahydro-2-naphthyl)-2,3-phenanthrenedicarboxylic anhydride, flat needles, m. 204-5°, characterized by dehydrogenation with Pd-C to 4-(2-naphthyl)-2,3-phenanthrenedicarboxylic anhydride (XIX), colorless needles, m. 264-5°, and identical with the anhydride prepared by the dimerization of VI; and dehydrogenation and **decarboxylation** of the derived Na salt of XIX gave II, m. 258-9°. Also cyclization of XIX gave the acid, **decarboxylated** and dehydrogenated to XII, red crystals, m. 238-9°, and identical with that previously prepared The combined mother liquors yielded more XIX and also some of the other isomer (XX). The Na salt of XX dehydrogenated and **decarboxylated** with powdered Cu and Pd-C to 1-(2-naphthyl)anthracene (XXI), colorless plates, m. 142-3°. The absorption spectrum of XXI showed absorption

bands for both anthracene and naphthalene and resembled that of 9,10-di-1-naphthylanthracene.

IT **855641-11-1**, 9-Phenanthrenepropionic acid, α,β-dibromo-
(preparation of)

RN 855641-11-1 HCAPLUS

CN 9-Phenanthrenepropionic acid, α,β-dibromo- (5CI) (CA INDEX NAME)



CC 10 (Organic Chemistry)

IT **Polymerization**
(dimerization, of arylpropiolic acids)

IT 192-40-5, Tetrabenzo[a,c,fg,op]naphthacene 192-77-8, 9H-Benzo[a]naphtho[1,2-g]fluorene 192-84-7, 9H-Benzo[b]naphtho[1,2-g]fluorene 193-09-9, Dibenzo[de,qr]naphthacene 197-70-6, Benzo[b]perylene 1985-37-1, 2,3-Naphthalenedicarboxylic anhydride, 1-phenyl- 4325-74-0, 1,2'-Binaphthyl 4325-78-4, Phenanthrene, 4-phenyl- 4444-28-4, [1,2'-Binaphthalene]-2,3-dicarboxylic anhydride 4843-42-9, 1-Naphthalenepropiolic acid 21532-73-0, Phenanthrene, 1-(1-naphthyl)- 35850-26-1, Phenanthrene, 4-(2-naphthyl)- 63041-47-4, 13H-Dibenzo[a,g]fluoren-13-one 67122-21-8, 4-Phenanthrol, 1,2,3,4-tetrahydro-4-phenyl- 67122-22-9, Phenanthrene, 1,2-dihydro-4-phenyl- 86853-93-2, 9H-Naphtho[2,1-c]fluoren-9-one 114468-92-7, 2,3-Phenanthrenedicarboxylic anhydride, 4-phenyl- 114469-09-9, 9H-Benzo[a]naphtho[1,2-g]fluoren-9-one 119925-43-8, Anthracene, 1-(2-naphthyl)- 133477-96-0, 2,3-Phenanthrenedicarboxylic anhydride, 1-(1-naphthyl)- 408320-46-7, Naphthalene, 6-ethynyl-1,2,3,4-tetrahydro- 408320-54-7, Naphthalene, 6-(1-chlorovinyl)-1,2,3,4-tetrahydro- 832732-96-4, 2,3-Anthracenedicarboxylic acid, 5,6,7,8-tetrahydro-1-(5,6,7,8-tetrahydro-2-naphthyl)-, sodium salt 855598-99-1, Phenanthrene, 1-(1-naphthyl)-, compound with 1,3,5-trinitrobenzene 855615-32-6, 2,3-Phenanthrenedicarboxylic anhydride, 5,6,7,8-tetrahydro-4-

(5,6,7,8-tetrahydro-2-naphthyl)- 855615-33-7, 2,3-Phenanthrenedicarboxylic anhydride, 4-(2-naphthyl)- **855641-11-1**, 9-Phenanthrenepropionic acid, α,β-dibromo- 855701-25-6, Phenanthrene, 1,6-dimethoxy- 855948-77-5, 2,3-Anthracenedicarboxylic anhydride, 5,6,7,8-tetrahydro-1-(5,6,7,8-tetrahydro-2-naphthyl)- 856067-88-4, 9H-Naphtho[2,1-c]fluorene-8-carboxylic acid, 9-oxo- 856199-80-9, 2-Naphthalenepropiolic acid, 5,6,7,8-tetrahydro- 857542-01-9, 9H-Benzo[a]naphtho[1,2-g]fluoren-9-one, oxime 857542-02-0, 7H-Benzo[c]naphtho[2,1-g]fluoren-7-one, oxime 857542-03-1, 7H-Benzo[c]naphtho[2,1-g]fluoren-7-one 857542-04-2, 9H-Benzo[a]naphtho[1,2-g]fluoren-9-ol 857542-06-4, 9H-Benzo[a]naphtho[1,2-g]fluorene-8-carboxylic acid, 9-oxo- 857542-08-6, 9H-Benzo[a]naphtho[1,2-g]fluorene-8-carboxylic acid, 1,2,3,4,10,11,12,13-octahydro-9-oxo- 857542-10-0, 7H-Benzo[c]naphtho[2,1-g]fluorene-6-carboxylic acid, 7-oxo- 858462-22-3, 2-Naphthaleneacrylic acid, α,β-dibromo-5,6,7,8-tetrahydro- 859331-97-8, Anthracene, 1-(2-naphthyl)-, compound with 1,3,5-trinitrobenzene 859745-61-2, 13H-Dibenzo[a,g]fluorene-12-carboxylic acid, 13-oxo- 859789-33-6, Triphenylene, 1-(9-phenanthryl)- 859789-44-9, 2,3-Triphenylenedicarboxylic anhydride, 1-(9-phenanthryl)- 860700-92-1, Benzo[b]perylene, compound with 1,3,5-trinitrobenzene
(preparation of)

L128 ANSWER 59 OF 60 HCAPLUS COPYRIGHT 2005 ACS on STN
1954:49390 Document No. 48:49390 Original Reference No. 48:8743b-i,8744a-i,8745a-i,8746a-d Synthesis and reactions of 1-methyl-2-vinyl-4-hydroxycyclohexene. Stork, Gilbert; Wagle, S. S.; Mukharji, P. C. (Harvard Univ.). Journal of the American Chemical Society, 75, 3197-204 (Unavailable) 1953. CODEN: JACSAT. ISSN: 0002-7863. OTHER SOURCES: CASREACT 48:49390.

GI For diagram(s), see printed CA Issue.

AB Pure 1-methyl-2-vinyl-4-hydroxycyclohexene (I), 1-methyl-2-vinylcyclohexene (II), and 6-methyl-1-vinylcyclohexene (III) have been prepared for the 1st time. I and II do not take part in the Diels-Alder reaction and previously described adducts of II (cf. Cook and Lawrence, C.A. 32, 2109.9; Robins and Walker, C.A. 46, 9545a; 47, 1118e) are in reality derived from III. 2,5-Me(MeO)C6H3CO2H (IV) (300 g.), 3 l. absolute EtOH, and 300 cc. concentrated H2SO4 refluxed 10 hrs., most of the EtOH distilled off, the residue diluted with H2O, extracted with Et2O, and the extract washed with aqueous NaHCO3 and H2O, dried, and distilled yielded 278 g. Et ester (V) of

IV, colorless oil, b5 125-35°. To 35 g. LiAlH4 in 3 l. dry Et2O was added 300 g. V at such a rate as to maintain gentle refluxing, the mixture refluxed 2 hrs., cooled, very carefully decomposed with saturated aqueous Na2SO4, the Et2O layer decanted off, the inorg. residue repeatedly extracted with Et2O, the combined Et2O extract and Et2O layer evaporated, and the residue distilled to give 220 g. 2,5-Me(MeO)C6H3CH2OH (VI), b0.6 104-6°. To 220 g. VI in 300 cc. Et2O was added dropwise with gentle stirring and cooling 250 g. SOCl2, the mixture let stand 6 hrs. in the cold, poured on ice, extracted with Et2O, and the extract washed with aqueous NaHCO3 and H2O, dried, and distilled to yield 150 g. 2,5-Me(MeO)C6H3CH2Cl (VII), b12 123-8°, m. 44-5° (from petr. ether, b. 20-40°).

VII (85 g.), 56 g. powdered KCN, and 200 g. freshly dried MeCN refluxed 16 hrs., the mixture cooled, filtered, the filter residue washed several times with Et2O, the washing combined with the filtrate, washed 4 times with H2O, dried with Drierite, evaporated, and the residual oil distilled gave 2,5-Me(MeO)C6H3CH2CN (VIII), m. 43-5° (from cyclohexane). VIII (90 g.) refluxed 16 hrs. with 180 g. KOH in 300 cc. H2O and 300 cc. EtOH, the resulting clear solution cooled, diluted with H2O, extracted with Et2O, and the aqueous solution filtered, cooled in ice, and carefully acidified with ice-cold dilute HCl gave 90 g. 2,5-Me(MeO)C6H3CH2CO2H (IX), white silky needles, m. 104° (from aqueous MeOH). IX (90 g.), 150 cc. dry C6H6, and 150 g. SOCl2 refluxed 4 hrs. on a steam bath, the solvent removed in vacuo, the residue diluted with C6H6, again evaporated in vacuo, this process repeated 3 times to remove the last traces of SOCl2, the resulting crude acid chloride slowly added with stirring and cooling to 75 g. 25% aqueous Me2NH, the mixture warmed to room temperature, stirred 16 hrs., extracted with Et2O, and the extract washed with H2O, dried, and evaporated gave 82 g. crude 2,5-Me(MeO)C6H3CH2CONMe2 (X); analytical sample, b0.5 142-3°. Crude X (82 g.) slowly dropped with stirring into a suspension of 16 g. LiAlH4 in 800 cc. dry Et2O, the mixture refluxed 4 hrs., cooled, decomposed with saturated aqueous Na2SO4, the clear supernatant Et2O layer decanted off, the inorg. residue extracted 4 times with Et2O, and the combined Et2O solution evaporated yielded 2,5-Me(MeO)C6H3CH2CH2NMe2 (XI), b0.7 90-2°; picrate, m.

162-3.5° (from EtOH). Na (12 g.) added slowly -50° in small pieces to 12 g. XI in 250 cc. liquid NH3 at and 30 cc. absolute EtOH, the mixture stirred about 5 hrs. at -40 to -50° until the blue color disappeared, evaporated overnight, hydrolyzed with H2O, extracted with Et2O, the extract washed with H2O, dried, evaporated, and the oily residue distilled gave 11 g. 1-(2-dimethylaminoethyl)-2-methyl-5-methoxy-1,4-cyclohexadiene (XII), b4 98-102°. To 10 g. XII was added with cooling and stirring in 1 portion 10 cc. ice-cold 15% HCl, the mixture treated after exactly 1 min. with stirring with 10 g. dry Na2CO3, the Et2O layer removed, the residual mass extracted with Et2O, and the combined Et2O solution dried with Na2SO4 and evaporated to give 9.4 g. crude 4-methyl-3-(2-dimethylaminoethyl)-3-cyclohexen-1-one (XIII), containing only traces of the Δ1-isomer; contact with the acid for more than 1 min. invariably resulted in appreciable amts. of the Δ1-isomer of XIII. Crude XIII (9.4 g.) slowly added with stirring to 2 g. LiAlH4 suspended in 250 cc. Et2O, the mixture stirred 1 hr. at room temperature, decomposed with vigorous stirring with saturated aqueous Na2SO4, treated with Na2SO4, the supernatant Et2O layer decanted off, the inorg. residue repeatedly washed with Et2O, and the combined Et2O solution dried and evaporated gave 9.0 g. 1-(2-dimethylaminoethyl)-2-methyl-5-hydroxycyclohexene (XIV), colorless liquid, b16 149-51°. To 20 g. XIV in 50 cc. dry C6H6 was gradually added with cooling and gentle stirring 25 g. MeI in 50 cc. C6H6, the mixture heated 0.5 hr. on the steam bath, treated again with 10 g. MeI in 25 cc. C6H6, heated 20 min., cooled, filtered, and the filter residue carefully washed several times with dry C6H6 and dried to give 34 g. crude XIV.MeI; analytical sample, m. 224° (decomposition) (from MeOH). XIV.MeI (25 g.) in 540 cc. MeOH and 60 cc. H2O stirred vigorously 10 hrs. with Ag2O freshly prepared from 159 g. AgNO8 and 3.8 g. NaOH, the mixture filtered, the inorg. residue washed with MeOH, the combined MeOH solution carefully concentrated to a small volume on the steam bath, the residue distilled. the distillate, b. 85-100°/2-4 mm., taken up in Et2O, washed with H2O, dried with Na2SO4, evaporated, and the residual oil distilled gave 6.6 g. I, b1.8 82-4°, λEtOHmax. 240 mμ, ε 18060; 3,5-dinitrobenzoate (86%), m. 88° (from cyclohexane). I on ozonolysis gave 27-8% CH2O, identified as its crystalline dimedon derivative, m. 187-9°. I refluxed with maleic anhydride or

p-benzoquinone in C6H6, or heated at 180° in a sealed tube with MeCH:CHCHO gave only polymers but no adducts. I (3 g.) in 5 cc. pyridine treated with 3 g. Ac2O in 5 cc. pyridine 8 hrs. at room temperature, the mixture poured on ice, extracted with Et2O, the Et2O extract washed with H2O, dilute ice-cold HCl, dilute ice-cold aqueous Na2CO3, and H2O, dried, evaporated, and the residue distilled gave 2 g. acetate (XV) of I, colorless mobile liquid, b0.7 79-81°. XV did not give a Diels-Alder adduct with maleic anhydride or MeCH:CHCHO. XIV (6 g.) added slowly with cooling to dry HCl in Et2O, the resulting white solid quickly filtered off, washed with dry Et2O, dissolved in 15 cc. CHCl3, the solution treated with 5 drops concentrated HCl and 15 cc. dihydropyran, the mixture let stand 5 hrs. at room temperature, washed twice with 10% aqueous NaOH and H2O, dried, evaporated, the residual oil distilled, the fraction b4 130-40° (3.6 g.) dissolved in 15 cc. dry C6H6, the solution treated with 5 g. MeI and again with 5 g. MeI after 20 min., heated 20 min. on the steam bath, cooled, evaporated in vacuo, the residual oil treated with freshly precipitated Ag2O in MeOH in the usual way, the resulting product heated in vacuo, and the distillate, b6 80-120°, redistd. under N gave 1.5 g. tetrahydropyran ether of I, b3 95-105°; analytical sample, b3 95-8°. To 6.9 g. I in 30 cc. pyridine was added with cooling 7.0 g. MeSO2Cl, the mixture let stand 45 min. at room temperature, poured on ice, and extracted with Et2O, the extract washed with H2O, ice-cold dilute HCl, ice-cold dilute aqueous Na2CO3, and H2O, dried, and evaporated, the resulting crude mesylate added dropwise with stirring to 4 g. LiAlH4 in 250 cc. dry Et2O, the solution refluxed 2 hrs., cooled, decomposed with saturated aqueous Na2SO4, and treated with solid Na2SO4, the Et2O layer decanted off, the residue extracted several times with Et2O, the combined Et2O solution dried, the Et2O distilled off under N, and the residual oil distilled to give 4.5 g. II, colorless liquid with a characteristic odor, b. 154-8°, λEtOHmax. 240 mμ, ε 16000. 2,6-Dimethylcyclohexanone (48 g.) and tert-AmOK (prepared from 18 g. K and 340 cc. tert-AmOH) added simultaneously during 1 hr. to 600 cc. Et2O previously saturated 2 hrs. with C2H2, the

solution vigorously stirred during the addition while C2H2 was passed, in the bubbling with C2H2 continued 4 hrs., the mixture let stand overnight at room temperature, decomposed with saturated aqueous NH4Cl, the Et2O layer washed with H2O, dried, evaporated, and the residual oil distilled gave 27 g. 2,6-dimethyl-1-ethynylcyclohexanol (XVI), colorless liquid, b25 92-5°, m 55° (from petr. ether, b. 30-60°). XVI (16 g.) reduced in the presence of 2% Pd-SrCO3 with 1 mole H gave 2,6-dimethyl-1-vinylcyclohexanol (XVII), b25 82-3°. XVII (10 g.) heated under N at 195-200° with 12 g. KHSO4, the distillate dried, distilled, and the fraction b. 164-8° redistd. gave 2,6-dimethyl-1-vinylcyclohexene, b. 165-6°, λEtOHmax. 238 mμ, ε 10350, did not form any adduct with maleic anhydride after prolonged refluxing in C6H6 in the presence of p-C6H4(OH)2, but was **polymerized.** C2H2 was bubbled 2 hrs. through 1000 cc. Et2O, the solution treated simultaneously during about 1.5 hrs. with 80 g. 2-methylcyclohexanone and tert-AmOK (from 32 g. K and 600 cc. tert-AmOH) while C2H2 was passed through the mixture, the bubbling with C2H2 continued 5 hrs., and the mixture let stand overnight and worked up in the usual manner to give 45 g. 2-methyl-1-ethynylcyclohexanol (XVIIA), b25 82-6°, which solidified immediately; the solid XVIIA dissolved with gentle warming in petr. ether (b. 30-60°) containing a little Et2O, the solution filtered, and the filtrate cooled deposited pure XVIIA, silky needles, m. 59° (from petr. ether); the mother liquors let stand 2 days deposited a 2nd small crop to give a total yield of 24 g. XVIIA; the residue after removal of the solid XVIIA yielded 18 g. epimeric XVIIA, b25 78-80°. Solid XVIIA (40 g.) reduced over 2% Pd-SrCO3 catalyst with 1 mole H yielded 36 g. 2-methyl-1-vinylcyclohexanol (XVIII), b30 76-7°. XVIII (16 g.) heated with 18 g. powdered KHSO4 under N at 190°, and the distillate dried with Na2SO4 and redistd. twice gave a diene (XIX), b. 156-7°, λEtOHmax. 233 mμ, ε 12310. XIX (6 g.) and 8 g. maleic anhydride in 50 cc. dry C6H6 refluxed overnight under N, the solution concentrated, diluted with Et2O, filtered, the filtrate washed several times with H2O, dried, evaporated, and the residue recrystd. 3 times from Et2O-petr. ether gave 0.6 g. adduct (XX), m. 113°. Liquid XVIIA similarly gave XIX, b. 154-6°, λEtOHmax. 233 mμ, ε 10000, which gave with maleic anhydride in C6H6 XX, m. 113°. 6-Methyl-1-cyclohexenecarboxylic acid (62 g.) in 450 cc. Et2O and 50 cc.

tetrahydrofuran added to 18 g. LiAlH4 in 600 cc. Et2O at a rate such as to maintain gentle refluxing, the solution refluxed 1 hr., cooled, the excess LiAlH4 destroyed with EtOAc, then with ice-cold dilute HCl, and the Et2O layer washed with H2O and dilute aqueous NaHCO3, dried, and distilled gave 42 g. 6-methyl-1-cyclohexen-1-ylcarbinol (XXI), colorless mobile liquid, b20 110-12°. To 56 g. XXI in 230 cc. petr. ether containing 5 cc. pyridine was added dropwise with stirring 99 g. PBr3 in 180 cc. petr. ether, the mixture warmed slowly to room temperature, let stand overnight, poured on ice, extracted with Et2O, and the extract worked up to give 60 g. 6-methyl-1-(2-bromoethyl)cyclohexene (XXII), b30 102-4°. CH2(CO2Et)2 (102 g.) added with ice cooling to 8.0 g. NaH in 400 cc. dry C6H6, the mixture let stand 2 hrs. at room temperature, heated 2 hrs. on the steam bath, cooled in ice, treated dropwise with shaking with 60 g. XXII, let stand overnight at room temperature, heated 10 hrs. on a steam bath, refluxed 3 hrs. in an oil bath, cooled to room temperature, poured into H2O, the C6H6 layer washed with H2O, evaporated, the residue distilled, and the distillate, b0.9 120-5°, redistd. yielded 78 g. Et 2-carbethoxy-3-(6-methyl-1-cyclohexen-1-yl)propionate (XXIII), colorless mobile liquid, b0.9 122-3°. XXIII (75 g.) added dropwise with stirring at 80° to 80 g. KOH in 50 cc. H2O during 1.5 hrs., the mixture heated 1 hr., the solution evaporated to dryness, the residue dissolved in 50 cc. H2O, the solution washed with Et2O, cooled in ice salt, decomposed with the calculated amount of ice-cold dilute HCl below 5°, the separated oil extracted with Et2O, the extract washed with H2O, dried, evaporated, the residual viscous liquid dried 0.5 hr. in vacuo **decarboxylated** 25 min. at 180°, and the residue distilled gave 43 g. 3-(6-methyl-1-cyclohexen-1-yl)propionic acid (XXIV), b0.6 114-16°; benzylthiuronium salt, m. 162°. XXIV carefully neutralized with the calculated amount of NaHCO3, the resulting Na salt dried overnight at 120°, powdered, a 19-g. aliquot suspended in 200 cc. dry C6H6, cooled in ice, treated with 1 drop pyridine and 20 g. (COCl)2, the mixture kept 1 hr. at 0° and 2 hrs. at room temperature, filtered, evaporated in vacuo at room temperature, the residue treated with 100 cc. C6H6, the C6H6 distilled off again, the residual acid chloride

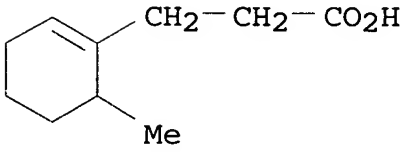
treated in 60 cc. Me2CO with stirring with 9 g. NaN3 in 24 cc. H2O below 5°, the mixture stirred 1 hr., the Me2CO layer evaporated in vacuo at room temperature, the residue in 100 cc. dry C6H6 heated gently 0.5 hr. on the steam bath, refluxed 15 min. after the N evolution ceased, the residual oily crude isocyanate (15 g.) added immediately to 15 g. LiAlH4 in 900 cc. dry Et2O, the mixture stirred overnight at room temperature, refluxed 4-5 hrs., cooled in ice, decomposed in the usual way, and worked up gave N-methyl-2-(6-methyl-1-cyclohexen-1-yl)ethylamine (XXV), b1.5 70°, colorless liquid with a characteristic odor, turned yellow on standing; phenylthiourea derivative, m. 78° (from C6H6-petr. ether). XXV (5 g.) and 7.5 g. HCO2Et heated 9 hrs. in a sealed tube at 150°, the resulting liquid heated on a steam bath in vacuo 1 hr. to remove the volatiles, the residual crude oily N-formyl derivative (10 g.) stirred 3 hrs. at room temperature with 5.2 g. LiAlH4 in 600 cc. Et2O, and the mixture refluxed 1 hr., cooled, decomposed, and worked up in the usual way gave N,N-dimethyl-2-(6-methyl-1-cyclohexen-1-yl)ethylamine (XXVI), colorless mobile oil, b2.5 72-4°; analytical sample, b2.5 70°. To 11 g. XXVI in 30 cc. C6H6 was added with stirring and cooling 15 g. MeI in 20 cc. C6H6, the mixture heated about 0.5 hr. on the steam bath, treated with 7.5 g. MeI in 20 cc. C6H6, again heated 20 min., cooled, diluted with petr. ether, and filtered, and the filter residue washed 3 times with petr. ether and dried in air to give 20.5 g. crude XXVI.MeI. Crude XXVI.MeI (20 g.) in 480 cc. MeOH containing 10% H2O treated with vigorous stirring with Ag2O prepared from 13 g. AgNO3 and 3.3 g. NaOH, the mixture stirred overnight, filtered, the inorg. residue washed 3 times with MeOH, the combined MeOH solution carefully concentrated on the steam bath, the residual viscous liquid heated in an oil bath (decomposition began at 150°), the distillate extracted with Et2O, the extract washed with H2O, dried, the Et2O evaporated in a stream of N, and the residual oil distilled under N gave 4.5 g. III, b. 155-8°; redistd., b. 156°, λEtOHmax. 232 mμ, ε 20000. III (2.5 g.) and 4 g. maleic anhydride in 25 cc. C6H6 heated 8 hrs. under N on a steam bath, the clear solution concentrated, diluted with Et2O, the Et2O solution washed several times with H2O, dried, concentrated, cooled, and the mixture

filtered gave 2.5 g. XXVII, m. 113°; an addnl. 0.5 g. was isolated from the mother liquors. The **infrared** absorption spectrum of I is recorded.

IT **408538-62-5**, 1-Cyclohexene-1-propionic acid, 6-methyl-
854725-03-4, 1-Cyclohexene-1-propionic acid, 6-methyl-, compound with 2-benzyl-2-thiopseudourea
(preparation of)

RN 408538-62-5 HCAPLUS

CN 1-Cyclohexene-1-propanoic acid, 6-methyl- (9CI) (CA INDEX NAME)



RN 854725-03-4 HCAPLUS

CN 1-Cyclohexene-1-propionic acid, 6-methyl-, compd. with 2-benzyl-2-thiopseudourea (5CI) (CA INDEX NAME)

CM 1

CRN 408538-62-5
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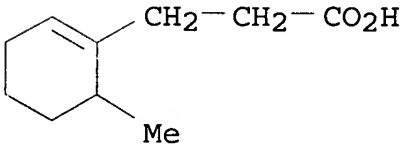

CM 2

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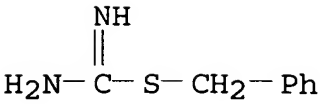

CC 10 (Organic Chemistry)
IT 629-09-4, Hexane, 1,6-diiodo- 6331-99-3, Cyclohexanol, 2-methyl-1-vinyl- 15564-30-4, Cyclohexanol, 1-ethynyl-2-methyl- 63649-33-2, Cyclohexanol, 1-ethynyl-2,6-dimethyl- 73502-04-2, Benzyl alcohol, 5-methoxy-2-methyl- 90416-25-4, Anisole, 3-(chloromethyl)-4-methyl- 92806-35-4, Acetic acid, (5-methoxy-o-tolyl)- 144711-50-2, Cyclohexene, 1-(bromomethyl)-6-methyl- 319457-53-9, 1-Cyclohexene-1-methanol, 6-methyl- 408507-35-7, 1-Cyclohexene-1-ethylamine, N,6-dimethyl- **408538-62-5**, 1-Cyclohexene-1-propionic acid, 6-methyl- 431059-53-9, 1-Cyclohexene-1-ethylamine, N,N,6-trimethyl- 854712-02-0, Cyclohexanol, 2,6-dimethyl-1-vinyl- 854718-40-4, Cyclohexene, 1,3-dimethyl-2-vinyl- 854724-25-7, 1-Cyclohexene-1-ethylamine, N,N,6-trimethyl-, picrate **854725-03-4**, 1-Cyclohexene-1-propionic acid, 6-methyl-, compound with 2-benzyl-2-thiopseudourea **854725-03-4**, Pseudourea, 2-benzyl-2-thio-, compound with 6-methyl-1-cyclohexene-1-propionic acid 854726-19-5, 3-Cyclohexen-1-ol, 3-(2-dimethylaminoethyl)-4-methyl- 854912-73-5, 2-Cyclohexen-1-one, 3-(2-dimethylaminoethyl)-4-methyl- 854913-05-6, 3-Cyclohexen-1-one, 3-(2-dimethylaminoethyl)-4-methyl- 855391-18-3, Phenethylamine, 5-methoxy-N,N,2-trimethyl- 855391-19-4, Phenethylamine, 5-methoxy-N,N,2-trimethyl-, picrate 855409-06-2, 1,4-Cyclohexadiene-1-ethylamine, 5-methoxy-N,N,2-trimethyl- 855949-35-8, m-Anisic acid, 6-methyl-, ethyl ester 856982-23-5, Propene, 3-chloro-, compound with maleic anhydride 857172-25-9, Ammonium, [2-(5-hydroxy-2-methyl-1-cyclohexen-1-yl)ethyl]trimethyl-, iodide 857476-49-4, Urea, 1-methyl-1-[2-(6-methyl-1-cyclohexen-1-yl)ethyl]-3-phenyl-2-thio- 857593-24-9, Ammonium, trimethyl[2-(6-methyl-1-cyclohexen-1-yl)ethyl]-, iodide 857946-34-0, Acetamide, 2-(5-methoxy-o-tolyl)-N,N-dimethyl- 858436-90-5, 1,2-Naphthalenedicarboxylic anhydride, 1,2,3,5,6,7,8,8a-octahydro-5-methyl- 860375-26-4, Malonic acid, (6-methyl-1-cyclohexen-1-ylmethyl)-, diethyl ester 861069-38-7, Acetonitrile, (5-methoxy-o-tolyl)-
(preparation of)

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1949:11226 Document No. 43:11226 Original Reference No.

43:2271e-i,2272a-i,2273a-i,2274a-b Biosynthesis of penicillins. III. Preparation and evaluation of precursors for new penicillins. Behrens, Otto K.; Corse, Joseph; Huff, Dorothea E.; Jones, Reuben G.; Soper, Quentin F.; Whitehead, Calvert W. Journal of Biological Chemistry, 175, 771-92 (Unavailable) 1948. CODEN: JBCHA3. ISSN: 0021-9258.

AB Methods are described for evaluation of compds. as precursors for new penicillins: (a) The ratio of units in the test container to units in control. Comparable results were obtained from P. notatum NRRL 1976 and P. chrysogenum Q-176. Stimulation may be interpreted as utilization of compound as a precursor. Lack of stimulation does not necessarily mean lack of utilization. (b) The ratio of antibacterial activity for Bacillus subtilis to that for Staphylococcus aureus compared with the same ratio using pure benzylpenicillin, which is defined as 1.0. (c) The relative position of the active portion in an adsorption column indicates a new penicillin. Culturing with N-2-hydroxyethyl-α-(allylmercapto)acetamide (I) deposited a new penicillin in a column. (d) The Craig method was used to determine the distribution coeffs. of the penicillins (C.A. 41, 6672i) formed between acid and ether. The penicillin formed using p-HSC6H4SCH2CO2H showed coeffs. and activities different from the controls while the activities and coeffs. with p-H2O3AsC6H4NHSO2C6H4SCH2CO2H-p as test precursor were similar to the controls. (e) Attempts were made to isolate the penicillin. With N-allyl-β-chloropropionamide as precursor the active material was recovered as the Na salt, 900 units/mg., distribution coefficient 0.64, but Cl in the product was below theory. β,β-Diphenylpropionic acid led to a penicillin, 1700 units/mg., coefficient 0.84, containing no diphenylpropionic group, but probably an aliphatic acyl group (UV absorption). Tryparsamide led to no As in the recovered penicillin; similarly, 2-thiophenecarboxylic acid and some derivs. were not utilized. Data obtained by these methods are presented for many compds. including aryl carboxylic acids, α-substituted phenylacetic acids, aliphatic acids, aryl aliphatic (other than acetic) acids, a miscellaneous unclassified group of acids, and derivs. of these acids. Preparation and some properties of new compds. in the above series are presented. Methods of preparation were: (A) The Schotten-Baumann method was applied to the acid chloride and the amino compound, allylamine, HOCH2CH2NH2, or DL-valine. (B) The Et or Me ester was heated with the amine. (C) EtSH (40 g.) was allowed to react with CH2:CHCO2Me (43 g.) in the presence of Triton B (2 drops) to form EtSCH2CH2CO2Me (61 g.), b55 109-13°. (D) CH2:CHCH2SCH2CONHCH2CH2OH (Soper, et al. J. Am.

Chemical Society 70, 2849-55(1948)) (53.0 g.) in 100 mL. Me2CO was treated with 33.0 mL. 30% H2O2 for 1 wk. N-2-hydroxyethyl-α-(allylsulfinyl)acetamide (II) was recrystd. from EtOAc or EtOAc-MeOH. (E) CH2:CHCH2SCH2CONHCH2CH2OH (44.5 g.) in 1 l. Me2CO with 75 mL. 30% H2O2 was allowed to stand 10 days yielding 47.4 g. of the sulfonyl compound (III), an orange oil. (F) Addition of CH2:CHCOOMe (100 g.) to 200 mL. CH2:CHCH2OH, in which was dissolved 5.3 g. Na, produced a **gelatinous** precipitate The mixture was heated 1 h., poured into water, and extracted with ether. The ether solution was dried and distilled, b65 116-32°, n20.5D, 1.4312, yield 50.3 g., mainly Me β-(allyloxy)propionate. The 2nd fraction b65 120-30°, n20.5D 1.4394, yield 23.5 g., was chiefly the allyl ester. (G) DL-Alanyl-DL-valine (Fischer and Scheibler, C.A. 3, 315) was treated with p-ClC6H4COCl and NaOH to give about 90% N-[N-(p-chlorobenzoyl)-DL-alanyl]-DL-valine (IV), m. 204-6° (from dilute EtOH). p-ClC6H4CO2H contaminant was removed by washing with ether. (H) CH.tplbond.CCMe2OH (Hurd and McPhee, C.A. 41, 4095g) (130 g.), CuO (10 g.), NH4Cl (5 g.) and concentrated HCl (225 mL.) were shaken together 0.5 h. below 40°, and the non-aqueous layer washed with HCl, dried, and fractionated to yield 34% CH.tplbond.CCMe2Cl, b. 77-9° (Favorskii and Favorskaya, C.A. 39, 3651.4). This compound (194 g.) was treated with malonic ester (330 g.) in 1 l. absolute alc. in which had been dissolved 46 g. Na, the mixture filtered, the alc. evaporated under vacuum, the residual sirup treated with dilute cold HCl, extracted with ether, the ether solution washed and dried, the ether evaporated, and the remaining liquid fractionated in vacuo through a Vigreux column to give 192 g. (45%) CH.tplbond.CCMe2CH(CO2Et)2, b3 102-4°; from this was derived 148 g. (98%) of the crystalline acid, m. 105-6°. The acid was **decarboxylated** by heating at 180-200° 1-2 h. to 85% CH.tplbond.CCMe2CH2CO2H (IVa), b2 75-7° (bath temperature 130°); Me ester b. 150-3°, 65% yield. (I) Chloroacetylvaline (9.4 g.) was added to 10 g. PhAsCl2 in 30 mL. 10 N NaOH (Quick and Adams, C.A. 16, 1560). After dilution, filtering, and acidification, an oil precipitated which on recrystn. from water gave 8.5 g. CHMe2CH(COOH)NHCOCH2.As(O2H)Ph (V), m. 188° (decomposition). (J) To the Grignard reagent from m-(CF3)C6H4Br, Mg, and

dry ether 0.15 g. powdered Se was added (Morgan and Porritt, C.A. 19, 3260) and the mixture hydrolyzed. After the ether layer was separated, washed, and extracted with 3 N NaOH, the resulting aqueous extract was added to 0.15 mol ClCH2CO2Na in 100 mL. water. In a few min. the mixture was acidified. Alternate extns. with ether and alkaline solution and acidification gave m-(CF3)C6H4SeCH2CO2H (Va) b7 140-2°, m. 58.5-9.5°. (K) Cl(CH2)3CN (52 g.), PhSH (56 g.), and NaOMe (28 g.) in 300 mL. absolute alc. was refluxed with stirring overnight. After the solvent was evaporated, the organic layer was washed and distilled in vacuo to give 72 g. impure PhS(CH2)3CN b0.1 135-7°; the acid obtained on hydrolysis m. 58-60°. (L) Br(CH2)4CO2Et, PhSH, and NaOEt in absolute alc. produced PhS(CH2)4CO2Et, b0.2 121-4°. (M) HO2C(CH2)4CO2Et (87 g.) with SOCl2 formed the chloride, which with PhCl, AlCl3, and CS2 gave 66.4 g. p-ClC6H4CO(CH2)4CO2Et, m. 59-60°; saponification with KOH gave the acid, m. 134-6°. Reduction with Zn and HCl in toluene-water, followed by treatment with MeOH resulted in p-ClC6H4(CH2)5CO2Me, b0.4 122-5°. (N) (p-ClC6H4)2CO was converted by the Reformatskii reaction to 90% (p-ClC6H4)2C(OH)CH2CO2Et, m. 96-7°, **dehydrated** by P2O5 in C6H6 and saponified to (p-ClC6H4)2C:CHCO2H, m. 173-4°. The acid was allowed to take up 0.10 mol H at 4 atmospheric over 5% Pd on C to yield 71% (p-ClC6H4)2CHCH2CO2H (VI), m. 182-3°. (O) Desoxyanisoin and BrCH2CO2Et in dry C6H6 was treated with Zn dust, the reaction mixture shaken with dilute H2SO4, the C6H6 layer separated and dried, and, after removal of the C6H6, the product distilled in vacuo with **dehydration** to 90% Et β,γ-bis(p-methoxyphenyl)butenoate, b2 221°; hydrogenation and saponification gave 90% β,γ-bis(p-methoxyphenyl)butyric acid (VII), m. 167-8°. Data on precursors are given in the order: acid, N-substituted amide, method of preparation (or taken from the literature or purchased com.), m.p. or b.p. of amide, stimulation (see Test a) of the amide (if no amide is given, value is for the acid): NCCH2CO2H, HOCH2CH2, B, oil, 0.9; ClCH2CH2CO2H, allyl, A, 39-40°, 1.0; HOCH2CH2CO2H, HOCH2CH2, B, 73.5-75, 1.0; γ,γ,γ-trichlorobutyric, DL-valine, A, 197, 1.0; CF3CH(OH)CH2CO2H, HOCH2CH2, B, 59-61, 1.1; CH2:CHCH2CO2H, HOCH2CH2, A, b1 138-42, 1.4; (ethylmercurimercapto)acetic, -, -, -, toxic; β-hydroxybutyric, HOCH2CH2, B, 68-71, 1.0; MeOCH2CH2CO2H, HOCH2CH2, B, b1.5 142-5, 1.0; 2-thiophenecarboxylic (VIII),

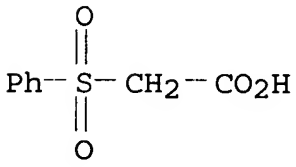
HOCH2CH2, B, 90-1, 1.0; VIII, allyl, A, 65, 1.0; VIII, DL-valine, A, 123-4, 1.0; allylsulfinylacetic, II, D, 81.5-82, 1.2; allylsulfonylacetic, III, E, oil, 0.9; EtSCH2CH2CO2H (C), HOCH2CH2, B, b0.45 173-5, 1.0; sorbic, HOCH2CH2, B, b1 158-60, 1.1; β-allyloxypropionic (F), HOCH2CH2, B, b0.3 142-4, 0.8; tert-butylacetic, DL-valine, A, 147-8, 0.8; isocaproic, DL-valine, A, 100-1, 1.0; γ-ethoxybutyric, HOCH2CH2, B, b1 138-40, 1.0; p-ClC6H4CO2H (IX), HOCH2CH2, A, 113-14, 1.0 (acid alone, 1.0); IX, allyl, A, 73, 1.0; IX, DL-valine, A, 178-9, 1.0; IX, DL-alanyl-DL-valine, G, 204-6, 1.0; BzOH (X), allyl, -, -, 0.9; X, 2-benzamido-1,3-propanediol, B, 67-9, 1.0; p-O:AsC6H4CH2CO2H, -, -, -, 1.0; PhCH2SO2H, DL-valine, A, 120-3, 1.0; IVa, (H), HOCH2CH2, B, b0.5 150-5, 0.8; cyclopentylacetic, HOCH2CH2, B, 57-8, 1.6; hexahydrobenzoic, DL-valine, A, 195-7, 1.0; BzCO2H, -, -, -, 1.0; mandelic, HOCH2CH2, B, 61-4, 1.0; PhSeCH2CO2H, HOCH2CH2, A, 56-8, 1.2 (acid alone, 1.8); PhSO2CH2CO2H, HOCH2CH2, B, 93-4, 1.1 (acid alone, 1.0); Ph(HO2)AsCH2CO2H, DL-valine, I, 188 (dec.), 1.0 (acid alone, toxic); C6H11CH2CO2H (XI), HOCH2CH2, B, 66-8, 1.0; XI, DL-valine, A, 178-9, 1.1; δ-carbethoxyvaleric, HOCH2CH2, A, oil, 1.0; PhC.tplbond.CCO2H, -, -, -, 0.9; NCCHPhCO2H, HOCH2CH2, B, 105-7, 0.8; Va, -, J, 58.5-9.5, 1.0; cinnamic (XII), HOCH2CH2, B, 101, 1.0; XII, DL-valine, A, 183-4, 1.0; XII, allyl, A, 90-2, 0.9; (2,4-dichlorobenzylsulfonyl)acetic, -, -, -, 0.9; PhCH(CO2H)2, bis(2-hydroxyethyl), B, oil, 1.2; (p-chlorobenzylsulfonyl)acetic, -, -, -, 0.9; hydrocinnamic, DL-valine, A, 141-3, 1.0; MeCH(SPh)CO2H, -, -, -, 1.3; PhSCH2CH2CO2H, DL-valine, A, 93-4, 1.1; MeOCHPhCO2H, HOCH2CH2, B, 84-7, 1.0; tropic, HOCH2CH2, B, oil, 1.2; PhCH2SO2CO2H, -, -, -, 1.0; N-phenylsarcosine, HOCH2CH2, B, 56-7, 1.0; (p-chlorocarbobenzoxy)glycine, -, -, 108-9.5, 1.0; γ-(2,4-dichlorophenoxy)butyric, -, -, -, toxic; styrylacetic, allyl, A, 61-3, 1.4; β-(p-bromophenyl)butyric, DL-valine, A, 134-5, 2.5; carbobenzoxyglycine, -, -, -, 1.2; γ-(p-nitrophenyl)butyric, DL-valine, A, 138-43, 1.5; EtCHPhCO2H, DL-valine, A, oil, 1.0; Me2CPhCO2H, DL-valine, A, oil, 1.1; β-phenylbutyric, HOCH2CH2, B, oil, 0.9; γ-phenylmercaptobutyric, -, K, 58-60, 2.0; γ-phenoxybutyric, HOCH2CH2, B, 70-2, 1.0; γ-(p-aminophenyl)butyric, DL-valine, obtained by catalytic hydrogenation of the nitro compound, 175-9, 0.8; fencholic, -, -, -, toxic; γ-cyclohexylbutyric, HOCH2CH2, B, 45-8, 1.1; capric, HOCH2CH2, -, 75, 1.0; 3-indolepropionic, -, -, -, 0.9; γ-benzoylbutyric, -, -, -, 1.0; benzylsuccinic, -, -, -, 1.0; γ-(p-bromophenyl)isovaleric, DL-valine, A, 109-10, 0.8; β-(p-chlorophenyl)isovaleric, -, -, -, 0.5; β-(p-fluorophenyl)isovaleric, -, -, -, 0.9; β-(p-iodophenyl)isovaleric, -, -, -, toxic;

β-(p-nitrophenyl)isovaleric, DL-valine, A, 110-15, 1.3; δ-phenylvaleric, DL-valine, A, 98-100, 0.8; δ-phenylmercaptovaleric (L), HOCH2CH2, B, 91-2, 1.0; β-(p-hydroxyphenyl)isovaleric, -, -, -, 1.0; β-(p-aminophenyl)isovaleric, -, -, -, 1.0; p-Me3SiC6H4SeCH2CO2H, -, -, b4 170-3, toxic; cyclohexylvaleric, -, -, -, toxic; 10-hendecenoic, HOCH2CH2, B, 66-7, 1.0; 3-indolebutyric, HOCH2CH2, B, oil, 1.0; ε-(p-chlorophenyl)caproic (M), HOCH2CH2, B, oil, 1.4; lauric, HOCH2CH2, B, 86-7, 0.9; 1-naphthalenepropionic, HOCH2CH2, B, 60-1, 1.0; 6-benzoyl-3-ketocaproic, -, -, -, 1.0; γ-mesitylbutyric, -, -, 82-4, toxic (acid); Ph2CHCO2H, HOCH2CH2, B, 118-19, 1.0; myristic, HOCH2CH2, B, 94-5, 1.0; VI (N), DL-valine, A, 155-6, 0.9 (acid alone 0.4); Ph2CHCH2CO2H, HOCH2CH2, B, 94, 0.9; 4-methoxy-1-naphthalenebutyric, HOCH2CH2, B, oil, 0.6; (PhCH2)2CHCO2H, HOCH2CH2, B, 83-4, 0.9; palmitic, HOCH2CH2, B, 97.5, 1.0; β,β-di-p-tolylpropionic, HOCH2CH2, B, 85-6, 0.9; 9-(p-iodophenyl)hendecanoic, HOCH2CH2, B, oil, 1.0; 3-phenylhendecanoic, HOCH2CH2, B, oil, 1.0; linoleic, HOCH2CH2, B, b1 215-20, 0.9; VII (O), DL-valine, A, 147-8, 1.0; ricinoleic, HOCH2CH2, B, 54-5, 1.0; 9,10-dihydroxystearic, HOCH2CH2, B, 150, 1.4; β-1-pyrenoylpropionic (C20H14O3), -, -, -, toxic.

IT **3959-23-7**, Acetic acid, (phenylsulfonyl)-
(in penicillin production)

RN 3959-23-7 HCAPLUS

CN Acetic acid, (phenylsulfonyl)- (6CI, 8CI, 9CI) (CA INDEX NAME)



CC 11C (Biological Chemistry: Microbiology)

IT 74-11-3, Benzoic acid, p-chloro- 94-82-6, Butyric acid, 4-(2,4-dichlorophenoxy)- 106-16-1, Ricinoleamide, N-2-hydroxyethyl- 142-58-5, Tetradecanamide, N-2-hydroxyethyl- 142-78-9, Dodecanamide, N-2-hydroxyethyl- 339-34-4, Hydrocinnamic acid, p-fluoro-β,β-dimethyl- 372-32-7, Butyramide, 4,4,4-trifluoro-3-hydroxy-N-2-hydroxyethyl- 512-77-6, Fencholic acid 544-31-0, Hexadecanamide, N-2-hydroxyethyl- 611-73-4, Glyoxylic acid, phenyl- 637-44-5, Propiolic acid, phenyl- 830-96-6, 3-Indolepropionic acid 884-33-3, Succinic acid, benzyl-

1138-80-3, Glycine, N-carboxy-, N-benzyl ester 1501-05-9, Butyric acid, 4-benzoyl- **3959-23-7**, Acetic acid, (phenylsulfonyl)- 5866-99-9, Benzamide, N-allyl-p-chloro- 5962-88-9, Cyclohexanevaleric acid 6961-46-2, Cinnamamide, N-2-hydroxyethyl- 6973-28-0, Valine, N-(benzylsulfonyl)- 7400-54-6, Benzamide, p-chloro-N-2-hydroxyethyl- 7499-60-7, 1-Pyrenebutyric acid, γ-oxo- 7726-08-1, Decanamide, N-2-hydroxyethyl- 10283-95-1, Benzamide, N-allyl- 10480-90-7, Crotonamide, N-2-hydroxyethyl- 13911-63-2, Arsinic acid, (carboxymethyl)phenyl- 13911-63-2, Acetic acid, phenylarsinico- 15029-40-0, Acetamide, 2-cyano-N-2-hydroxyethyl- 17431-94-6, Propionic acid, 2-(phenylthio)- 17893-46-8, Acetic acid, (phenylselenyl)- 17983-69-6, Silane, [p-(carboxymethylselenyl)phenyl]trimethyl- 17983-69-6, Acetic acid, [p-(trimethylsilyl)phenylselenyl]- 20545-92-0, 10-Undecenamide, N-2-hydroxyethyl- 21957-67-5, Valine, N-hydrocinnamoyl- 23054-51-5, Valeric acid, 5-(2-hydroxyethylcarbamoyl)-, ethyl ester 23917-33-1, Propionamide, N-2-hydroxyethyl-3,3-diphenyl- 28203-59-0, Acetic acid, (benzylsulfonyl)- 30186-06-2, Butyric acid, 4-mesityl- 35544-45-7, Propionamide, N-2-hydroxyethyl-3-methoxy- 41041-34-3, Cinnamamide, N-allyl- 42288-16-4, Hydrocinnamic acid, p-chloro-β,β-dimethyl- 51816-47-8, Butyramide, N-2-hydroxyethyl-4-phenoxy- 52845-23-5, Hydracrylamide, N-2-hydroxyethyl- 63122-37-2, 2-Thiophenecarboxamide, N-allyl- 68171-52-8, Linoleamide, N-2-hydroxyethyl- 73040-35-4, 3-Indolebutyramide, N-2-hydroxyethyl- 93008-37-8, Acetamide, N-2-hydroxyethyl-2,2-diphenyl- 93448-78-3, 2-Thiophenecarboxamide, N-2-hydroxyethyl- 93505-87-4, Benzyl alcohol, p-chloro-, (carboxymethyl)carbamate 93505-87-4, Glycine, N-carboxy-, p-chlorobenzyl ester 93709-63-8, Valine, N-p-chlorobenzoyl- 118528-57-7, Valine, N-cyclohexylcarbonyl- 138625-63-5, Benzamide, N-[2-hydroxy-1-(hydroxymethylethyl]- 139882-33-0, Acetamide, 2-cyano-N-2-hydroxyethyl-2-phenyl- 177270-08-5, Valine, N-cinnamoyl- 223409-84-5, 3-Butenamide, N-allyl-4-phenyl- 228402-73-1, Valine, N-3,3-dimethylbutyryl- 300700-02-1, Acetic acid, (2,4-dichlorobenzylsulfonyl)- 784189-22-6, Acetamide, 2-(allylthio)-N-2-hydroxyethyl- 836610-57-2, Acetamide, N-2-hydroxyethyl-2-(phenylsulfonyl)- 848743-99-7, Valine, N-(β,β-dimethyl-p-nitrohydrocinnamoyl)- 854007-21-9, 2-Thiophenecarboxamide, N-(1-carboxy-2-methylpropyl)- 854731-13-8, Cyclopentaneacetamide, N-2-hydroxyethyl- 855414-77-6, Cyclohexaneacetamide, N-2-hydroxyethyl- 855424-58-7, Cyclohexanebutyramide, N-2-hydroxyethyl- 855475-70-6, 4-Pentynamide, N-2-hydroxyethyl-3,3-dimethyl- 855660-91-2, Mandelamide, N-2-hydroxyethyl- 855907-06-1, Hexanamide,

6-(p-chlorophenyl)-N-2-hydroxyethyl- 855912-65-1, Hexanoic acid, 6-benzoyl-3-oxo- 855928-82-4, Acetamide, N-2-hydroxyethyl-2-(phenylselenyl)- 855934-41-7, Acetic acid, (ethylmercurithio)- 856199-59-2, 1-Naphthalenepropionamide, N-2-hydroxyethyl- 856984-14-0, Propionamide, 3-(allyloxy)-N-2-hydroxyethyl- 857479-06-2, Valeramide, N-2-hydroxyethyl-5-(phenylthio)- 857768-61-7, Hydracrylamide, N-2-hydroxyethyl-2-phenyl- 857943-05-6, Propionamide, N-2-hydroxyethyl-3,3-di-p-tolyl- 858214-02-5, Hydrocinnamamide, N-2-hydroxyethyl-β-methyl- 858214-57-0, Hydrocinnamamide, 2-benzyl-N-2-hydroxyethyl- 858814-12-7, Butyramide, 3-hydroxy-N-2-hydroxyethyl- 859056-99-8, Propionamide, 3-(ethylthio)-N-2-hydroxyethyl- 859324-80-4, Undecanamide, N-2-hydroxyethyl-9-(p-iodophenyl)- 859800-42-3, Phenaceturic acid, α-isopropyl-δ,δ-dimethyl- 859985-10-7, 1-Naphthalenebutyramide, N-2-hydroxyethyl-4-methoxy- 860374-08-9, Malonamide, N,N'-bis(2-hydroxyethyl)-2-phenyl- 860417-09-0, Sorbamide, N-2-hydroxyethyl- 861053-22-7, Butyramide, 4-ethoxy-N-2-hydroxyethyl- 861058-57-3, Acetamide, N-2-hydroxyethyl-2-N-methylanilino- 861058-61-9, Acetamide, N-2-hydroxyethyl-2-methoxy-2-phenyl-
(in penicillin production)

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